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Screening Pilot Study of Fruit Seed Compositions by GC-MS and Their Potential Scenario Anti ACE2 and 2rh1 Receptors as a Recycling Possibility in the Coronavirus Pandemic

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Abstract

Background: Since 2019, several critical effects of the coronavirus pandemic have surfaced, including its psychological problems such as depression. The World Health Organization has approved a group of drugs and vaccines. However, the world still faces novel coronavirus mutations, requiring more ideas to investigate a drug, vaccine and phytochemical potential chemoprevention proposal. Severe Acute Respiratory Syndrome-Coronavirus (SARS-CoV)-2 co-operates directly with the Angiotensin-Converting Enzyme 2 (ACE2) to penetrate the target cells.

Aims: We aim to introduce the possibility of studying seed oil extract as an anti-depression, anti-stress, anti-epinephrine receptor (PDB: 2rh1) and as potentially binding anti-angiotensin-converting enzyme 2 (ACE2) agent.

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Methods and Methodology: We analyze the constituents of the six studied seeds' oil with Gas Chromatography-Mass Spectrometry (GC-MS) by performing an AutoDock analysis of the components' potential ligands to both the 2rh1 and ACE2.

Results: We observe convenient binding conformations between the investigated receptors and the 44 phytoconstituents. The AutoDock outcomes of the seeds' phytochemical GC-MS separated components reveal highly binding energy, with ACE2 higher than 2rh1.

Conclusion: The studied seed oil contains binding energy with currently studied receptors and molecular weight, which enables it to be studied in the future as a nanoparticle against viruses, vaccines and psychiatric drugs.

Keywords

Coronavirus; Depression; Seed Oil; Adrenaline; Angiotensin-Converting Enzyme 2; Autodock; Phytochemicals; Nanoparticles

Introduction

Fruit processing produces a significant quantity of wastes. The stones of fruits such as grapes (*Vitis vinifera*), plum (*Prunus* subg. *Prunus*: *Mirabelles*), apple (*Malus domestica*), Ajwa dates (*Phoenix dactylifera* L), pomegranate (*Punica granatum*) and avocado (*Persea Americana*) are the remains that are generally discarded as trash and can cause environmental problems [1,2]. Examining such underutilized wastes' likely dietary and therapeutic potentials will also diminish the desirable environmental waste load such as river water toxicity. Seed composition depends on maturation, the environmental cultivation state and extraction protocol method that makes about 6 to 20% of the seed oil as fatty acid, vitamin and phytosterol. The seed oil compositions vary between fatty acids (oleic, palmitic, stearic, linoleic acid), vitamins (isomers tocopherol) and phytosterol (stigmasterol), according to the method of extraction [3,4].

Recently, the global coronavirus (COVID-19) pandemic has drawn scientists' attention to the study of possible vaccines, herb and drug treatments and protection-potential medications [5,6]. The insertion of coronavirus into susceptible cells is complicated and needs some effort to assume the receptor-binding and proteolytic mechanism of virus-cell fusion. Coronaviruses (SARS-CoV) co-operate directly with the Angiotensin-Converting Enzyme 2 (ACE2) to penetrate the target. Studies showed that ACE2 is expressed in the mouth, tongue and lower lungs on type I and II alveolar epithelial cells, promoting viral insertions in the host [6,7]. The previous mechanism helps infuse SARS-CoV-2 entry, exploits the endogenous transcriptional machinery of alveolar cells to replicate it and spreads it into the entire lung and body, where ACE2 is expressed in other organs, including the kidney, heart and gut [5-7].

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ACE-1 and ACE-2 result in cleaving angiotensin peptides into angiotensin I (Ang 1) and generating angiotensin (Ang) II. Ang II has an inflammatory response that causes vasoconstriction, bronchoconstriction, increases vascular permeability and fibrosis. These previous action responses enhance Acute Respiratory Disease Syndrome (ARDS) and lung failure in patients infected with SARS-CoV-2 and that is different to the receptor number from one individual to another.

Carboxypeptidase (zinc metalloprotease) is known as ACE2, degrading Ang II to an anti-inflammatory Ang (1-7). Ang II's conversion to Ang (1-7) by the enzyme ACE2 produces effects that oppose the Ang II-mediated action. The SARS-CoV-2 virus infects alveolar pneumocytes by binding to ACE2, leading to a decrease in Ang II conversion to ACE2-derived peptides; for instance, a reduction in Ang (1-7) and its anti-inflammatory effects prevent the effects of Ang II and led to a higher imbalance between ACE1 and ACE2. The disturbance starts a storm of an inflammatory reaction and thus, the immune response will be overcome [6,8].

Although some animal studies proposed that the application of ACEIs could provide the inhibition of and treatment for the consequences of the COVID-19 infection, different scenarios indicate that their use may increase the infection's deleterious conditions. Therefore, more trials need to provide evidence of their effectiveness. The potential benefit-risk study of the traditional drugs and herb extracts during COVID-19 connected with other issues such as hypertension, heart failure and gut, colon and renal disease associated with diabetes should also be discussed. Further, the psychiatric consequences during the COVID-19 pandemic should be taken into consideration [5].

A previous study reported that the coronavirus (COVID-19) pandemic produced significant distress to patients with chronic illnesses, including the emotional state and perception, especially among patients with inflammatory bowel diseases [9].

Our previous study reported that dietary intake of vitamins, especially B6, B9 and B12 and herb extracts such as agarwood significantly affect mood and stress and decrease inflammation through β_2 adrenoreceptor (2rh1) binding energy [10]. Moreover, the combination of the beta-adrenergic receptor block and renin-angiotensin system inhibition throughout diminished the Ang II-induced inflammatory cascade reaction and increased Ang (1-7) as well as its anti-inflammatory effects [11-13].

We hypothesize that the seed oil extract can affect both receptors and have a potential beneficial effect in decreasing the entry of viruses in the human body, decreasing storm inflammatory outcomes and improving the mood, thus decreasing stress in the COVID-19 pandemic. From this point of view, we aim to study seed oil extract as an anti-depression, anti-stress and anti-epinephrine receptor (PDB: 2rh1) ACE2.

Material and Methods

Plant Study

Plant Materials

We obtained grape (*Vitis vinifera*), plum (*Prunus subg. Prunus: Mirabelles*), apple (*Malus domestic*), Ajwa dates (*Phoenix dactylifera L*), pomegranate (*Punica granatum*) and avocado (*Persea Americana*) seeds from fruits that were collected from a local market in Saudi Arabia for this study. Here, supplementary Fig. 1 shows the experimental design. Seeds were crushed in the crushing machine and extracted with a solvent (1: 5 w/v), where the solvent compositions were hexane and ethanol (1:1). After being soaked in the solvent for 10 minutes at room temperature ($28 \pm 2^\circ\text{C}$), the extracts were separately concentrated with a 40-50°C rotary evaporator 14-23. The ground seeds extracted independently with (n-hexane: absolute ethanol) as (1:1) yielded 6%, 35%, 5%, 21%, 15% and 68% oil, respectively and named as GSO (Grapes (*Vitis vinifera*) extracts), PSO (Plum (*Prunus subg. Prunus: Mirabelles*) extracts), ASO (Apple (*Malus domestic*) extracts), AWSO (Ajwa dates (*Phoenix dactylifera L*) extracts), PGSO (Pomegranate (*Punica granatum*) extracts), AVSO (Avocado (*Persea Americana*) extracts).

Figure 1: Experimental design. *Abbreviations: GSO: Grapes (*Vitis vinifera*) extracts; PSO: Plum (*Prunus subg. Prunus: Mirabelles*) extracts; ASO: Apple (*Malus domestic*) extracts; AWSO: Ajwa dates (*Phoenix dactylifera L*) extracts; PGSO: Pomegranate (*Punica granatum*) extracts; AVSO: Avocado (*Persea Americana*) extracts; GC-MS: Gas Chromatography-Mass Spectrometry; 2RH1: Epinephrine receptor; ACE2: Angiotensin-converting enzyme 2.

Gas Chromatography-Mass Spectrometry Analysis

We followed our previous method for the Gas Chromatography-Mass Spectrometry (GC-MS) analysis to separate the chemical constituents of the extract using a gas chromatography system (G3440B, Agilent Technologies, USA) [24].

The seeds extracts were re-dissolved in ethanol and filtered using a nylon 0.45 μm pore size membrane filter separately. The GC-MS analysis was performed using a general screening method [24]. The separation column was from Thermo Fisher Scientific (TR-5MS) and had the following properties: 30 m length, Internal Diameter (ID) 0.25 mm and film thickness 0.25 μm . The carrier gas was helium and the flow rate was 1 ml/min. A total of 2 μl of each sample was injected into splitless mode at an injection port with a temperature of 260°C. The GC thermal program started at 80°C and was conducted for 1.5 min. Next, the thermal program increased at the first ramp to 210°C at a rate of 30°C/min and then the rate was slowed to 20°C/min to reach the final temperature of 320°C; this temperature was held for 11 min. The ion source in MS was Electron Ionization (EI) and the analysis was conducted in a scanning mode with an electron energy of 70 eV. The ion source and transfer line temperatures were adjusted to 230°C. The composites of the plant extract were identified by computer explorations in the commercial libraries of Wiley and NIST (National Institute of Standards and Technology).

We then searched the Wiley and NIST mass spectral libraries to identify the chemical components of the seeds extract [24]. Furthermore, we screened the unique seed extracts separately for components with AutoDock to determine their potential as ligands of the anti-epinephrine receptor (PDB: 2rh1) and ACE2 to provide more convincing proof of the therapeutic opportunities provided by GSO, PSO, ASO, AWSO, PGSO and AVSO [25,26].

Autodock Analysis

Preparation of the modelled epinephrine receptor (PDB: 2rh1), Angiotensin-Converting Enzyme 2 (ACE2) and specific GSO, PSO, ASO, AWSO, PGSO and AVSO components for docking

The AutoDock Vina 4.2 software includes procedures for optimizing proteins and ligands, such as allowing atomic charges to make proteins more polar [26-29]. Proteins and ligands were adjusted through the charge and rotatable bond authorization, consideration of the energy contribution of desolvation through the binding of a ligand to the protein and previous naming of grid maps of the protein surface for synergy ligands by the auto grid. These tools increase the speed and accuracy of docking with a unique scoring capacity, optimize effectively and perform the multithreading of the molecular docking [26-29].

Result and Discussion

GC-MS Analysis Outcomes

The GC-MS analysis identified the chemical composition of GSO, PSO, ASO, AWSO, PGSO and AVSO extracts. The specific components that are unique to the extract are presented in Table 1-6, which include the chemical name, molecular weight, retention time and area percentage. Besides, Table 7 illustrates the results of the GC-MS chromatogram of the selected compounds in the studied seeds, namely, GSO, PSO, ASO, AWSO, PGSO and AVSO.

Area	Name	Formula	Mass (DB)	Base Peak	RT	Score (Lib)	CAS	Library
1153381	9-Octadecenamide, (Z)-	C18H35NO	281.3	59	14.014	96.01	301-02-0	NIST11.L
553719	9-Octadecenamide, (Z)-	C18H35NO	281.3	59	14.068	95.12	301-02-0	NIST11.L
312347	9-Octadecenamide, (Z)-	C18H35NO	281.3	59	14.132	80.8	301-02-0	NIST11.L
253901	Stigmastan-3,5-diene	C29H48	396.4	396.4	19.823	82.64	1000214-16-4	NIST11.L
196415	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	C19H34O2	294.3	81.1	12.335	88.67	112-63-0	NIST11.L
163338	Oleamide	C18H35NO	281	59	15.137	69.43	301-02-0	SWGDRUG.L
159068	9-Octadecenoic acid (Z)-, methyl ester	C19H36O2	296.3	55	12.367	79.86	112-62-9	NIST11.L
151791	Stigmastan-3,5-diene	C29H48	396.4	145.1	18.24	70.76	1000214-16-4	NIST11.L
122124	Hexadecanamide	C16H33NO	255.3	59	12.944	86.69	629-54-9	NIST11.L
117526	Phosphoric acid, trimethyl ester	C3H9O4P	140	110	3.274	90.14	512-56-1	NIST11.L
85055	Dodecyl acrylate	C15H28O2	240.2	55	9.575	89.7	2156-97-0	NIST11.L
61663	Pentanoic acid, 5-hydroxy-, 2,4-di-t-butylphenyl esters	C19H30O3	306.2	191.2	8.28	61.18	166273-38-7	NIST11.L
59729	Methyl stearate	C19H38O2	298.3	74	12.501	73.68	112-61-8	NIST11.L
46671	1-Pentadecyne	C15H28	208.2	55	12.736	75.63	765-13-9	NIST11.L
45722	Hexadecanoic acid, methyl ester	C17H34O2	270.3	74	11.217	88.84	112-39-0	NIST11.L
32926	11,13-Dimethyl-12-tetradecen-1-ol acetate	C18H34O2	282.3	207	14.656	65.15	1000130-81-0	NIST11.L
32557	4-Methyl-2,4-bis(4'-trimethylsilyloxyphenyl)pentene-1	C24H36O2Si2	412.2	207	21.984	60.24	1000283-56-8	NIST11.L
25237	1,3-Benzenediol, o-(4-methylbenzoyl)-o'-(2-methoxybenzoyl)-	C22H18O5	362.1	135.1	5.67	80.17	1000330-77-7	NIST11.L

20103	2-Bromotetradecane	C ₁₄ H ₂₉ Br	276.1	71.1	9.543	71.68	74036-95-6	NIST11.L
12553	Cyclotrisiloxane, hexamethyl-	C ₆ H ₁₈ O ₃ Si ₃	222.1	207	17.443	62.3	541-05-9	NIST11.L
11645	Isooctyl mercaptopropionate 3-	C ₁₁ H ₂₂ O ₂ S	218.1	57	11.907	66.69	30374-01-7	NIST11.L

Table 1: Results of the GC-MS analysis of the Grape Seed Extract (GSO).

Area	Name	Formula	Score	Mass (DB)	Base Peak	RT	CAS	Library
1754219	9-Octadecenamide, (Z) ⁻	C ₁₈ H ₃₅ NO	95.39	281.3	59	14.014	301-02-0	NIST11.L
837978	9-Octadecenamide, (Z) ⁻	C ₁₈ H ₃₅ NO	94.8	281.3	59	14.073	301-02-0	NIST11.L
412230	9,12-Octadecadienoic acid (Z,Z) ⁻	C ₁₈ H ₃₂ O ₂	74.12	280.2	55	12.709	60-33-3	NIST11.L
354051	Octadecanamide	C ₁₈ H ₃₇ NO	82.57	283.3	59	14.132	124-26-5	NIST11.L
336429	9-Octadecenoic acid, methyl ester, (E) ⁻	C ₁₉ H ₃₆ O ₂	91.3	296.3	55	12.367	1937-62-8	NIST11.L
335665	9-Octadecenamide, (Z) ⁻	C ₁₈ H ₃₅ NO	76.36	281.3	59	15.137	301-02-0	NIST11.L
295258	Benzamide, N-(1,3-dihydro-2-oxo-4-isobenzofuryl) ⁻	C ₁₅ H ₁₁ NO ₃	67.17	253.1	105	3.563	1000270-36-9	NIST11.L
248784	Squalene	C ₃₀ H ₅₀	88.57	410.4	69.1	16.539	111-02-4	NIST11.L
201429	Hexadecanamide	C ₁₆ H ₃₃ NO	88.56	255.3	59	12.944	629-54-9	NIST11.L
200337	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	C ₁₉ H ₃₄ O ₂	90.13	294.3	81.1	12.335	112-63-0	NIST11.L
196440	Dodecyl acrylate	C ₁₅ H ₂₈ O ₂	89.05	240.2	55	9.575	2156-97-0	NIST11.L
133468	Stigmastan-3,5-diene	C ₂₉ H ₄₈	70.87	396.4	396.4	19.817	1000214-16-4	NIST11.L
103286	cis-11-Hexadecenal	C ₁₆ H ₃₀ O	72.19	238.2	55	14.271	53939-28-9	NIST11.L
99402	Pentanoic acid, 5-hydroxy-, 2,4-di- <i>t</i> -butylphenyl esters	C ₁₉ H ₃₀ O ₃	64.7	306.2	191.2	8.275	166273-38-7	NIST11.L
90774	Oleamide	C ₁₈ H ₃₅ NO	68.81	281	59	16.474	301-02-0	SWGDRUG.L
80042	Stigmastan-3,5-diene	C ₂₉ H ₄₈	61.13	396.4	207	18.245	1000214-16-4	NIST11.L
71117	Hexadecane	C ₁₆ H ₃₄	60.94	226.3	71.1	7.874	544-76-3	NIST11.L

70968	Propanoic acid, 3-mercapto-, dodecyl ester	C15H30O2S	81.54	274.2	57.1	11.901	6380-71-8	NIST11.L
62331	Methyl stearate	C19H38O2	80.22	298.3	74	12.5	112-61-8	NIST11.L
59517	1,3-Benzenediol, o-(4-methylbenzoyl)-o'-(2-methoxybenzoyl)-	C22H18O5	80.78	362.1	135.1	5.676	1000330-77-7	NIST11.L
56219	Hexadecanoic acid, methyl ester	C17H34O2	88.83	270.3	74	11.217	112-39-0	NIST11.L
53892	1,2-15,16-Diepoxyhexadecane	C16H30O2	64.14	254.2	67	14.528	1000192-65-0	NIST11.L
45286	Dodecane, 1-iodo-	C12H25I	73.33	296.1	71.1	9.543	4292-19-7	NIST11.L
41330	Oxalic acid, cyclobutyl octadecyl ester	C24H44O4	64.72	396.3	55	13.554	1000309-70-8	NIST11.L
31933	(R)-(-)-14-Methyl-8-hexadecyn-1-ol	C17H32O	73.75	252.2	67	12.912	64566-18-3	NIST11.L
28347	11,13-Dimethyl-12-tetradecen-1-ol acetate	C18H34O2	66.06	282.3	207	14.656	1000130-81-0	NIST11.L
21037	Cyclotrisiloxane, hexamethyl-	C6H18O3Si3	61.01	222.1	207	29.14	541-05-9	NIST11.L

Table 2: Results of the GC-MS analysis of the Plum Seed Extract (PSO).

Area	Name	Formula	Score	Mass (DB)	Base Peak	RT	CAS	Library
6889234	9-Octadecenamide, (Z) ⁻	C18H35NO	94.13	281.3	59	14.03	301-02-0	NIST11.L
2945751	9-Octadecenamide, (Z) ⁻	C18H35NO	93.78	281.3	59	14.089	301-02-0	NIST11.L
1033287	cis-Vaccenic acid	C18H34O2	88.05	282.3	55.1	12.688	506-17-2	NIST11.L
1008732	9-Octadecenamide, (Z) ⁻	C18H35NO	86.69	281.3	59	14.142	301-02-0	NIST11.L
954396	cis-11-Eicosenamide	C20H39NO	88.97	309.3	59	15.143	10436-08-5	NIST11.L
610895	Hexadecanamide	C16H33NO	90.15	255.3	59	12.95	629-54-9	NIST11.L
593475	cis-11-Eicosenamide	C20H39NO	89.3	309.3	59	15.175	10436-08-5	NIST11.L
388532	Benzoic acid	C7H6O2	90.25	122	105	5.456	65-85-0	NIST11.L
323156	9-Octadecenoic acid (Z) ⁻ , methyl ester	C19H36O2	94.1	296.3	55	12.367	112-62-9	NIST11.L
267970	13-Docosenamide, (Z) ⁻	C22H43NO	83.16	337.3	59	16.48	112-84-5	NIST11.L
240133	Squalene	C30H50	83.22	410.4	69.1	16.539	111-02-4	NIST11.L
220504	9,12-Octadecadienoic acid (Z,Z) ⁻ , methyl ester	C19H34O2	85.99	294.3	55.1	12.34	112-63-0	NIST11.L
166826	2-pyrrolidinovalerophenone	C15H21NO	61.27	231.2	126	4.483	1000379-01-6	NIST11.L
160890	9,12-Octadecadienoic acid (Z,Z) ⁻	C18H32O2	80.2	280.2	55	12.843	60-33-3	NIST11.L

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156823	2-Furancarboxaldehyde, 5-methyl-	C ₆ H ₆ O ₂	68.01	110	110	3.568	620-02-0	NIST11.L
149932	2,5,5-Trimethyl-3-hexyn-2-ol	C ₉ H ₁₆ O	62.81	140.1	125.1	4.173	1522-16-3	NIST11.L
149396	dl-.alpha.-Tocopherol	C ₂₉ H ₅₀ O ₂	84.28	430.4	165.1	20.026	10191-41-0	NIST11.L
148913	13-Tetradecenal	C ₁₄ H ₂₆ O	69.47	210.2	55	14.271	85896-31-7	NIST11.L
145902	Dodecyl acrylate	C ₁₅ H ₂₈ O ₂	77.77	240.2	55	9.575	2156-97-0	NIST11.L
134293	9-Octadecenamide, (Z)-	C ₁₈ H ₃₅ NO	71.12	281.3	59	15.26	301-02-0	NIST11.L
115541	Phosphoric acid, trimethyl ester	C ₃ H ₉ O ₄ P	76.47	140	110	3.269	512-56-1	NIST11.L
114363	9-Octadecenoic acid (Z)-, methyl ester	C ₁₉ H ₃₆ O ₂	87.2	296.3	55	12.393	112-62-9	NIST11.L
104507	9,12-Octadecadienoic acid (Z,Z)-, phenylmethyl ester	C ₂₅ H ₃₈ O ₂	68.52	370.3	91.1	16.314	47557-83-5	NIST11.L
99081	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	C ₆ H ₈ O ₄	78.5	144	43	5.109	28564-83-2	NIST11.L
89982	7-Decen-1-ol acetate	C ₁₂ H ₂₂ O ₂	65.77	198.2	198.1	10.58	1000130-98-7	NIST11.L
73813	13-Octadecenal, (Z)-	C ₁₈ H ₃₄ O	74.15	266.3	55	13.554	58594-45-9	NIST11.L

Table 3: Results of the GC-MS analysis of the Apple Seed Extract (ASO).

Area	Name	Formula	Score	Mass (DB)	Base Peak	RT	CAS	Library
11938939	5-Hydroxymethylfurfural	C ₆ H ₆ O ₃	93.69	126	97	5.981	67-47-0	NIST11.L
7187956	9-Octadecenamide, (Z)-	C ₁₈ H ₃₅ NO	93.41	281.3	59	14.036	301-02-0	NIST11.L
2795712	Oleic Acid	C ₁₈ H ₃₄ O ₂	89.41	282.3	55.1	12.688	112-80-1	NIST11.L
2786153	9-Octadecenamide, (Z)-	C ₁₈ H ₃₅ NO	92.81	281.3	59	14.089	301-02-0	NIST11.L
1941282	5-Methyl-2-pyrazinylmethanol	C ₆ H ₈ N ₂ O	71.12	124.1	95	4.526	61892-95-3	NIST11.L
1755089	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	C ₆ H ₈ O ₄	85.74	144	144.1	5.13	28564-83-2	NIST11.L
1340413	9-Octadecenamide, (Z)-	C ₁₈ H ₃₅ NO	85.7	281.3	59	14.143	301-02-0	NIST11.L
1137031	cis-11-Eicosenamide	C ₂₀ H ₃₉ NO	88.05	309.3	59	15.143	10436-08-5	NIST11.L
1010531	Hexadecanamide	C ₁₆ H ₃₃ NO	89.11	255.3	59	12.955	629-54-9	NIST11.L
913214	.alpha.-D-Glucopyranoside, O-.alpha.-D-glucopyranosyl-	C ₁₈ H ₃₂ O ₁₆	68.86	504.2	60	8.575	597-12-6	NIST11.L

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	(1.fwdarw.3)-.beta.-D-fructofuranosyl							
523476	Dodecanoic acid	C12H24O2	62.4	200.2	101	7.232	143-07-7	NIST11.L
519466	Palmitic Acid	C16H32O2	82.97	256	73	11.554	57-10-3	SWGDRUG.L
464464	2,4-Dimethyl-3-pentanol acetate	C9H18O2	68.65	158.1	115.1	4.938	84612-74-8	NIST11.L
454918	.alpha.-D-Glucopyranoside, O-.alpha.-D-glucopyranosyl-(1.fwdarw.3)-.beta.-D-fructofuranosyl	C18H32O16	62.2	504.2	97	6.751	597-12-6	NIST11.L
445645	d-Glycero-l-gluco-heptose	C7H14O7	69.94	210.1	73	9.457	1000130-14-6	NIST11.L
422390	7-Methyl-Z-tetradecen-1-ol acetate	C17H32O2	60.7	268.2	71	7.516	1000130-99-6	NIST11.L
384795	Dodecanoic acid	C12H24O2	62.21	200.2	97	7.088	143-07-7	NIST11.L
343639	.alpha.-D-Glucopyranoside, O-.alpha.-D-glucopyranosyl-(1.fwdarw.3)-.beta.-D-fructofuranosyl	C18H32O16	69.04	504.2	43	4.226	597-12-6	NIST11.L
338707	9-Octadecenoic acid (Z), methyl ester	C19H36O2	93.39	296.3	55.1	12.367	112-62-9	NIST11.L
306881	Levoglucosenone	C6H6O3	74.73	126	98	4.836	37112-31-5	NIST11.L
275232	13-Docosenamide, (Z)	C22H43NO	82.89	337.3	59	16.48	112-84-5	NIST11.L
261583	Squalene	C30H50	74.99	410.4	69.1	16.539	111-02-4	NIST11.L
243810	Cyclopropanecarboxylic acid, 3-formyl-2,2-dimethyl-, ethyl ester	C9H14O3	68.54	170.1	141.1	6.371	66692-75-9	NIST11.L
229093	7,10-Octadecadienoic acid, methyl ester	C19H34O2	86.45	294.3	55.1	12.34	56554-24-6	NIST11.L
194471	Stigmastan-3,5-diene	C29H48	79.33	396.4	396.4	19.828	1000214-16-4	NIST11.L
180044	1H-Inden-1-ol, 2,3-dihydro-	C9H10O	66.21	134.1	133.1	5.815	#####	NIST11.L
166539	Phenol, 2,6-bis(1,1-dimethylethyl)-	C14H22O	64.8	206.2	191.2	8.27	128-39-2	NIST11.L
144137	Dodecanoic acid, 3-hydroxy-	C12H24O3	75.86	216.2	73	9.58	1883-13-2	NIST11.L
135632	Stigmastan-3,5-diene	C29H48	71.22	396.4	145.1	18.245	1000214-16-4	NIST11.L
129752	Chloro(2-methyloxiran-2-yl)acetic acid, t-butyl ester	C9H15ClO3	63.1	206.1	57	5.676	1000195-30-2	NIST11.L
129419	9-Octadecenamide, (Z)	C18H35NO	73.1	281.3	59	15.26	301-02-0	NIST11.L

124757	7-Methyl-Z-tetradecen-1-ol acetate	C17H32O2	67.8	268.2	109	11.907	1000130-99-6	NIST11.L
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Table 4: Results of the GC-MS analysis of the AJWA DATE SEED EXTRACT (AWSO).

Area	Name	Formula	Score	Mass (DB)	Base Peak	RT	CAS	Library
7881254	9-Octadecenamide, (Z)-	C18H35NO	94.13	281.3	59	14.035	301-02-0	NIST11.L
3678871	9-Octadecenamide, (Z)-	C18H35NO	93.57	281.3	59	14.094	301-02-0	NIST11.L
2484499	Squalene	C30H50	94.66	410.4	69.1	16.544	111-02-4	NIST11.L
1890724	.gamma.-Tocopherol	C28H48O2	94.32	416.4	416.4	19.052	7616-22-0	NIST11.L
1614995	Octadecanamide	C18H37NO	87.45	283.3	59	14.142	124-26-5	NIST11.L
1306538	cis-11-Eicosenamide	C20H39NO	86.97	309.3	59	15.143	10436-08-5	NIST11.L
851742	cis-11-Eicosenamide	C20H39NO	86.97	309.3	59	15.18	10436-08-5	NIST11.L
809801	Hexadecanamide	C16H33NO	91.31	255.3	59	12.95	629-54-9	NIST11.L
731639	13-Docosenamide, (Z)-	C22H43NO	93.29	337.3	59	16.48	112-84-5	NIST11.L
670773	5-Hydroxymethylfurfural	C6H6O3	78.42	126	97	5.815	67-47-0	NIST11.L
329977	9,12-Octadecadienoic acid (Z,Z)-	C18H32O2	83.51	280.2	55	12.688	60-33-3	NIST11.L
259024	Stigmastan-3,5-diene	C29H48	82.99	396.4	396.4	19.823	1000214-16-4	NIST11.L
236786	9-Octadecenamide, (Z)-	C18H35NO	72.37	281.3	59	15.26	301-02-0	NIST11.L
183380	9-Octadecenoic acid, methyl ester, (E)-	C19H36O2	90.67	296.3	55.1	12.367	1937-62-8	NIST11.L
177775	Stigmastan-3,5-diene	C29H48	71.73	396.4	145.1	18.245	1000214-16-4	NIST11.L
155592	Dodecyl acrylate	C15H28O2	86.06	240.2	55	9.58	2156-97-0	NIST11.L
136483	7-Hexadecenal, (Z)-	C16H30O	74.64	238.2	55	13.554	56797-40-1	NIST11.L
132310	Oleamide	C18H35NO	76.78	281	59	14.271	301-02-0	SWGDRUG.L
127624	Pentanoic acid, 5-hydroxy-, 2,4-di-t-butylphenyl esters	C19H30O3	65.87	306.2	191.2	8.27	166273-38-7	NIST11.L
122878	Oleanitrile	C18H33N	88.92	263.3	55	12.334	1000308-88-1	NIST11.L
121687	Octadecanoic acid	C18H36O2	77.44	284.3	55	12.843	57-11-4	NIST11.L
98579	n-Hexadecanoic acid	C16H32O2	75.86	256.2	73	11.554	57-10-3	NIST11.L
88320	Erucic Acid	C22H42O2	73.59	338	55.1	14.656	112-86-7	SWGDRUG.L

Table 5: Results of the GC-MS analysis of the Pomegranate Seed Extract (PGSO).

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Area	Name	Formula	Score	Mass (DB)	Base Peak	RT	CAS	Library
2897082	Cyclodecacyclododecene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18-octadecahydro-	C20H36	69.15	276.3	94.1	12.297	14113-80-5	NIST11.L
2811595	9-Octadecenamide, (Z)-	C18H35NO	93.38	281.3	59	14.02	301-02-0	NIST11.L
2745454	2H-Pyran, 2-(7-heptadecynyloxy)tetrahydro-	C22H40O2	80.95	336.3	81.1	12.891	56599-50-9	NIST11.L
2319924	E,Z-3,13-Octadecadien-1-ol acetate	C20H36O2	80.52	308.3	81.1	10.372	1000130-91-2	NIST11.L
1680890	1-Hexadecyn-3-ol, 3,7,11,15-tetramethyl-	C20H38O	73	294.3	69	13.11	29171-23-1	NIST11.L
1357304	Androstan-17-one, 3-ethyl-3-hydroxy-, (5.alpha.)-	C21H34O2	80.78	318.3	94.1	13.351	57344-99-7	NIST11.L
1283909	Z,E-2,13-Octadecadien-1-ol	C18H34O	76.45	266.3	85	13.581	1000131-10-3	NIST11.L
1250645	Cyclodecacyclododecene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18-octadecahydro-	C20H36	81.34	276.3	94	11.752	14113-80-5	NIST11.L
1092568	Chrysene, octadecahydro-	C18H30	75.03	246.2	94.1	10.923	2090-14-4	NIST11.L
1058031	9-Octadecenamide, (Z)-	C18H35NO	92.94	281.3	59	14.078	301-02-0	NIST11.L
1009366	9-Octadecenamide, (Z)-	C18H35NO	83.68	281.3	59	14.137	301-02-0	NIST11.L
849953	cis-11-Eicosenamide	C20H39NO	83.93	309.3	59	15.143	10436-08-5	NIST11.L
782505	Bicyclo[10.8.0]eicosane, (E)-	C20H38	75.55	278.3	81	11.789	1000155-85-0	NIST11.L
674421	Hexadecanamide	C16H33NO	68.87	255.3	69	12.95	629-54-9	NIST11.L
592928	dl- α -Tocopherol	C29H50O2	94.47	430.4	430.4	20.026	10191-41-0	NIST11.L
559398	Bicyclo[10.6.0]octadeca-1(12),15-diene	C18H30	82.51	246.2	94.1	10.334	1000155-85-1	NIST11.L
558452	Formic acid, 3,7,11-trimethyl-1,6,10-dodecatrien-3-yl ester	C16H26O2	74.54	250.2	121	13.779	1000132-11-0	NIST11.L
540335	cis-10-Nonadecenoic acid	C19H36O2	76.96	296.3	85.1	14.699	73033-09-7	NIST11.L
517071	Bicyclo[10.6.0]octadeca-1(12),15-diene	C18H30	79.35	246.2	81.1	10.596	1000155-85-1	NIST11.L
504483	Farnesol isomer a	C15H26O	80.22	222.2	69	13.297	1000108-92-4	NIST11.L
486502	3-Chloropropionic acid, heptadecyl ester	C20H39ClO2	86.52	346.3	55	9.58	1000283-05-1	NIST11.L

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445890	Z,Z-4,6-Nonadecadien-1-ol acetate	C21H38 O2	74.05	322.3	95.1	13.971	1000131- 08-4	NIST11 .L
438822	cis-9-Hexadecenoic acid, trimethylsilyl ester	C19H38 O2Si	66.59	326.3	117	13.709	1000333- 19-8	NIST11 .L
422108	2H-Pyran, 2-(7-heptadecynyloxy)tetrahydro-	C22H40 O2	82.98	336.3	85.1	15.715	56599- 50-9	NIST11 .L
372034	9,12-Octadecadienoic acid (Z,Z)-	C18H32 O2	81.92	280.2	55	12.709	60-33-3	NIST11 .L
345493	2H-Pyran, 2-(7-dodecynyloxy)tetrahydro-	C17H30 O2	74.06	266.2	85	14.586	16695- 32-2	NIST11 .L
319949	12-Methyl-E,E-2,13-octadecadien-1-ol	C19H36 O	77.79	280.3	69	14.276	1000130- 90-4	NIST11 .L
308267	1-Heptatriacotanol	C37H76 O	81.96	536.6	95.1	16.148	105794- 58-9	NIST11 .L
267929	Oleic Acid	C18H34 O2	70.63	282.3	55	11.538	112-80-1	NIST11 .L
251122	Stigmastan-3,5-diene	C29H48	83.63	396.4	396. 4	19.828	1000214- 16-4	NIST11 .L
227979	Cyclodecacyclotetradecene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20-eicosahydro-	C22H40	76.61	304.3	94	13.517	14113- 62-3	NIST11 .L
225643	9-Cycloheptadecen-1-one, (Z)-	C17H30 O	74.34	250.2	81.1	10.409	542-46-1	NIST11 .L
224112	12-Methyl-E,E-2,13-octadecadien-1-ol	C19H36 O	80	280.3	85	14.544	1000130- 90-4	NIST11 .L
220290	9,12,15-Octadecatrienoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl]ethyl ester, (Z,Z,Z)-	C25H40 O6	67.89	436.3	117	13.667	55320- 01-9	NIST11 .L
217000	Phenol, 2-undecyl-	C17H28 O	76.37	248.2	94.1	10.955	20056- 71-7	NIST11 .L
214629	E,E,Z-1,3,12-Nonadecatriene-5,14-diol	C19H34 O2	73.79	294.3	111. 1	14.94	1000131- 11-4	NIST11 .L
201901	cis-9-Hexadecenal	C16H30 O	80.37	238.2	97.1	11.447	56219- 04-6	NIST11 .L
197393	13-Docosenamide, (Z)-	C22H43 NO	77.49	337.3	59	16.48	112-84-5	NIST11 .L
196079	Caryophyllene oxide	C15H24 O	75.62	220.2	133. 1	12.565	1139-30- 6	NIST11 .L
174210	2-Acetoxy-1,1,10-trimethyl-6,9-epidioxydecalin	C15H24 O4	76.87	268.2	85	13.469	108511- 84-8	NIST11 .L
173866	9-Octadecenoic acid (Z)-, methyl ester	C19H36 O2	84.25	296.3	55	12.367	112-62-9	NIST11 .L
158247	Sclaral (sclareolide lactol)	C16H28 O2	70.48	252.2	237. 2	14.886	52811- 62-8	NIST11 .L
148648	2-Isoamylpyrazine	C9H14N 2	68.98	150.1	94.1	12.089	40790- 22-5	NIST11 .L

144711	.gamma.-Tocopherol	C28H48 O2	66.81	416.4	151. 1	19.047	7616-22- 0	NIST11 .L
130975	p-Menth-8-en-3-ol, acetate	C12H20 O2	71.42	196.1	121	12.522	89-49-6	NIST11 .L
127798	Farnesol isomer a	C15H26 O	74.05	222.2	69	13.014	1000108- 92-4	NIST11 .L
121571	Hexadecanoic acid, methyl ester	C17H34 O2	60.81	270.3	74	11.222	112-39-0	NIST11 .L
119991	Scleral (sclareolide lactol)	C16H28 O2	74.41	252.2	237. 2	14.635	52811- 62-8	NIST11 .L
118782	11,13-Dimethyl-12-tetradecen-1-ol acetate	C18H34 O2	70.73	282.3	69.1	16.539	1000130- 81-0	NIST11 .L
117278	Oleic Acid	C18H34 O2	71.31	282.3	55	11.639	112-80-1	NIST11 .L
114475	2-Acetoxy-1,1,10-trimethyl-6,9-epidioxydecalin	C15H24 O4	75.39	268.2	85	15.608	108511- 84-8	NIST11 .L
104445	2-Acetoxy-1,1,10-trimethyl-6,9-epidioxydecalin	C15H24 O4	72.68	268.2	59	15.26	108511- 84-8	NIST11 .L
102635	12-Methyl-E,E-2,13-octadecadien-1-ol	C19H36 O	73.38	280.3	43	14.779	1000130- 90-4	NIST11 .L
97105	12-Methyl-E,E-2,13-octadecadien-1-ol	C19H36 O	74.25	280.3	85.1	15.528	1000130- 90-4	NIST11 .L
95395	11,13-Dimethyl-12-tetradecen-1-ol acetate	C18H34 O2	69.81	282.3	57.1	16.758	1000130- 81-0	NIST11 .L
90205	Formic acid, 3,7,11-trimethyl-1,6,10-dodecatrien-3-yl ester	C16H26 O2	64.55	250.2	117	13.886	1000132- 11-0	NIST11 .L
83029	9,12-Octadecadienoic acid (Z,Z), methyl ester	C19H34 O2	82.86	294.3	94	12.335	112-63-0	NIST11 .L
81266	Stigmastan-3,5-diene	C29H48	62.42	396.4	207	19.352	1000214- 16-4	NIST11 .L
80710	7-Methyl-Z-tetradecen-1-ol acetate	C17H32 O2	73.25	268.2	117	13.843	1000130- 99-6	NIST11 .L
79895	Cyclohexane, 1,5-diethenyl-2,3-dimethyl-, (1.alpha.,2.beta.,3.beta.,5.beta.)-	C12H20	66.11	164.2	94	10.693	68779- 12-4	NIST11 .L
79553	Caryophyllene oxide	C15H24 O	80.12	220.2	95	13.174	1139-30- 6	NIST11 .L
75917	Heptacosane	C27H56	67.85	380.4	57	17.475	593-49-7	NIST11 .L
68591	Phenol, 2,5-bis(1,1-dimethylethyl)-	C14H22 O	60.78	206.2	191. 2	8.27	5875-45- 6	NIST11 .L
67261	Propanoic acid, 3-mercapto-, dodecyl ester	C15H30 O2S	78.73	274.2	57.1	11.901	6380-71- 8	NIST11 .L
67173	2-Acetoxy-1,1,10-trimethyl-6,9-epidioxydecalin	C15H24 O4	77.39	268.2	85.1	13.42	108511- 84-8	NIST11 .L
63628	2-Bromotetradecane	C14H29 Br	72.05	276.1	71.1	9.543	74036- 95-6	NIST11 .L

62123	1,2-15,16-Diepoxyhexadecane	C16H30 O2	77.92	254.2	69.1	13.046	1000192- 65-0	NIST11 .L
61775	1,2-15,16-Diepoxyhexadecane	C16H30 O2	74.2	254.2	97.1	9.997	1000192- 65-0	NIST11 .L
60013	12-Methyl-E,E-2,13-octadecadien-1-ol	C19H36 O	81.12	280.3	95	14.335	1000130- 90-4	NIST11 .L
59523	Heptacosane	C27H56	66.66	380.4	57	17.234	593-49-7	NIST11 .L
57603	Phosphoric acid, trimethyl ester	C3H9O4 P	87.9	140	110	3.279	512-56-1	NIST11 .L
56870	7-Hexadecenal, (Z)-	C16H30 O	74.19	238.2	57.1	12.217	56797- 40-1	NIST11 .L
50564	Heptacosane	C27H56	75.64	380.4	71.1	15.929	593-49-7	NIST11 .L
49635	2-methyltetracosane	C25H52	79.82	352.4	43	11.04	1000376- 72-6	NIST11 .L
44135	2-methyltetracosane	C25H52	76.32	352.4	71.1	11.083	1000376- 72-6	NIST11 .L
42262	3H-3,10a-Methano-1,2-benzodioxocin-3- ol, octahydro-7,7-dimethyl-, (3.alpha.,6a.beta.,10a.beta.)-	C13H22 O3	66.26	226.2	81	10.447	95906- 83-5	NIST11 .L
41762	(2,2,6-Trimethyl-bicyclo[4.1.0]hept-1-yl)- methanol	C11H20 O	67.8	168.2	94	10.73	78996- 11-9	NIST11 .L
41510	11,13-Dimethyl-12-tetradecen-1-ol acetate	C18H34 O2	63.75	282.3	57	16.341	1000130- 81-0	NIST11 .L
41096	1,2-15,16-Diepoxyhexadecane	C16H30 O2	77.5	254.2	69	13.207	1000192- 65-0	NIST11 .L
39859	Tricyclo[4.3.0.0(7,9)]nonane, 2,2,5,5,8,8- hexamethyl-, (1.alpha.,6.beta.,7.alpha.,9.alpha.)-	C15H26	64.69	206.2	81	10.27	54832- 82-5	NIST11 .L
33905	11,13-Dimethyl-12-tetradecen-1-ol acetate	C18H34 O2	76.72	282.3	69.1	15.383	1000130- 81-0	NIST11 .L
31812	2-Bromotetradecane	C14H29 Br	64.58	276.1	71.1	9.874	74036- 95-6	NIST11 .L
29097	11,13-Dimethyl-12-tetradecen-1-ol acetate	C18H34 O2	71.69	282.3	57	18.662	1000130- 81-0	NIST11 .L

*Notes for Tables 1-7: RT: Retention times (minutes); PA: peak area (%).

GC-MS analysis was carried for the Hexane: ethanoic (1:1) extracts applying Agilent Technologies (G3440B, USA).

The components of plant extract were characterized by computer simulations in commercial libraries of Wiley and NIST (National Institute of Standards and Technology).

The CAS number is a database index to identifying a given chemical

GSO: Grape (*Vitis vinifera*) extracts; PSO: Plum (*Prunus* subg. *Prunus*: Mirabelles) extracts; ASO: Apple (*Malus domestica*) extracts; AWSO: Ajwa dates (*Phoenix dactylifera* L) extracts; PGSO: Pomegranate (*Punica granatum*) extracts; AVSO: Avocado (*Persea Americana*) extracts

Table 6: Results of the GC-MS analysis of the Avocado Seed Extract (AVSO).

Compounds	Chemical (PubChem CID:)	GC MS SPECTRA(Chromatogram)
9-Octadecenamide, (Z)- Or Oleamide Present in all(GSO, PSO, ASO, AWSO, PGSO, AVSO)	Compound CID: 5283387 MF: C₁₈H₃₅NO MW: 281.5g/mol InChIKey: FATBGEAMYMYZAF-KTKRTIGZSA-N IUPAC Name: (Z)-octadec-9-enamide Create Date: 2005-03-27
Stigmastan-3,5-diene Present in (GSO, PSO, AWSO, PGSO, AVSO)	Compound CID: 525918 MF: C ₂₉ H ₄₈ MW: 396.7g/mol InChIKey: ICCTZARHLGPHMT-UHFFFAOYSA-N IUPAC Name: 17-(5-ethyl-6-methylheptan-2-yl)-10,13-dimethyl-2,7,8,9,11,12,14,15,16,17-decahydro-1H-cyclopenta[a]phenanthrene Create Date: 2005-03-27
Hexadecanamide Present in all(GSO, PSO, ASO, AWSO, PGSO, AVSO)	Compound CID: 69421 MF: C₁₆H₃₃NO MW: 255.44g/mol InChIKey: HSEMFIWZXHQJAE-UHFFFAOYSA-N IUPAC Name: hexadecanamide Create Date: 2005-03-26

Compounds	Chemical (PubChem CID:)	GC MS SPECTRA(Chromatogram)
Pentanoic acid, 5-hydroxy-, 2,4-di-tert-butylphenyl esters Present in GSO, PSO, PGSO	Compound CID: 605777 MF: C ₁₉ H ₃₀ O ₃ MW: 306.4g/mol InChIKey: ZUILXYOZKNAZSJ-UHFFFAOYSA-N IUPAC Name: (2,4-ditert-butylphenyl) 5-hydroxypentanoate Create Date: 2005-03-27
Methyl stearate GSO, PSO ONLY	Compound CID: 8201 MF: C ₁₉ H ₃₈ O ₂ MW: 298.5g/mol InChIKey: HPEUJPJOZXNMSJ-UHFFFAOYSA-N IUPAC Name: methyl octadecanoate Create Date: 2005-03-26
4-Methyl-2,4-bis(4'-trimethylsilyloxyphenyl)pentene-1 Present in GSO, PSO, ONLY	Compound CID: 610040 MF: C₂₄H₃₆O₂Si₂ MW: 412.7g/mol InChIKey: YCRIXHKHAODKFH-UHFFFAOYSA-N IUPAC Name: trimethyl-[4-[2-methyl-4-(4-trimethylsilyloxyphenyl)pent-4-en-2-yl]phenoxy]silane Create Date: 2005-03-27

Compounds	Chemical (PubChem CID:)	GC MS SPECTRA(Chromatogram)
1,3-Benzenediol, o-(4-methylbenzoyl)-o'-(2-methoxybenzoyl)- Present in GSO, PSO ,ONLY	Compound CID: 91715040 MF: C ₂₂ H ₁₈ O ₅ MW: 362.4g/mol InChIKey: YKAUQBZMUPNUKE-UHFFFAOYSA-N IUPAC Name: [3-(4-methylbenzoyl)oxyphenyl] 2-methoxybenzoate Create Date: 2015-04-28
2-Bromotetradecane GSO, AVSO ONLY	Compound CID: 12798926 MF: C₁₄H₂₉Br MW: 277.28g/mol InChIKey: WZGQIDWFBFDMLE-UHFFFAOYSA-N IUPAC Name: 2-bromotetradecane Create Date: 2007-02-08
Cyclotrisiloxane, hexamethyl- Present in GSO, PSO ,ONLY	Compound CID: 10914 MF: C ₆ H ₁₈ O ₃ Si ₃ MW: 222.46g/mol InChIKey: HTDJPCNNEPUOOQ-UHFFFAOYSA-N IUPAC Name: 2,2,4,4,6,6-hexamethyl-1,3,5,2,4,6-trioxatrisilinane Create Date: 2005-03-27

Compounds	Chemical (PubChem CID:)	GC MS SPECTRA(Chromatogram)
Isooctyl 3-mercaptopropionate GSO ONLY	Compound CID: 104386 MF: C₁₁H₂₂O₂S MW: 218.36g/mol InChIKey: ZHUWXKIPGGZJNW-UHFFFAOYSA-N IUPAC Name: 6-methylheptyl 3-sulfanylpropanoate Create Date: 2005-03-26
Squalene Present in(PSO, ASO, AWSO, PGSO, AVSO	Compound CID: 638072 MF: C₃₀H₅₀ MW: 410.7g/mol InChIKey: YYGNTYWPHWGJRM-AAJYLUCBSA-N IUPAC Name: (6E,10E,14E,18E)-2,6,10,15,19,23-hexamethyltetracos-2,6,10,14,18,22-hexaene Create Date: 2004-09-16
Propanoic acid, 3-mercapto-, dodecyl ester Present in GSO, AVSO	Compound CID: 80796 MF: C₁₅H₃₀O₂S MW: 274.5g/mol InChIKey: ARNIBHATWCFFIK-UHFFFAOYSA-N IUPAC Name: dodecyl 3-sulfanylpropanoate Create Date: 2005-03-26

Compounds	Chemical (PubChem CID:)	GC MS SPECTRA(Chromatogram)
1,2-15,16-Diepoxyhexadecane	<p>Compound CID: 543423</p> <p>MF: C₁₆H₃₀O₂</p> <p>MW: 254.41g/mol</p> <p>InChIKey: KHOGZDMZNQXOFX-UHFFFAOYSA-N</p> <p>IUPAC Name: 2-[12-(oxiran-2-yl)dodecyl]oxirane</p> <p>Create Date: 2005-03-27</p>
cis-Vaccenic acid ASO ONLY	<p>Compound CID: 5282761</p> <p>MF: C₁₈H₃₄O₂</p> <p>MW: 282.5g/mol</p> <p>InChIKey: UWHZIFQPPBDJPM-FPLPWBNSA-N</p> <p>IUPAC Name: (Z)-octadec-11-enoic acid</p> <p>Create Date: 2004-09-16</p>
cis-11-Eicosenamide Present in (ASO, AWSO, PGSO, AVSO)	<p>Compound CID: 5365374</p> <p>MF: C₂₀H₃₉NO</p> <p>MW: 309.5g/mol</p> <p>InChIKey: LBHQTVBKPMHICN-KTKRTIGZSA-N</p> <p>IUPAC Name: (Z)-icos-11-enamide</p> <p>Create Date: 2005-03-27</p>

Compounds	Chemical (PubChem CID:)	GC MS SPECTRA(Chromatogram)
2-Furancarboxaldehyde, 5-methyl- Present in (ASO)only	Compound CID: 12097 MF: C₆H₆O₂ MW: 110.11g/mol InChIKey: OUDFNZMQXZILJD-UHFFFAOYSA-N IUPAC Name: 5-methylfuran-2-carbaldehyde Create Date: 2005-03-27
dl-α-Tocopherol Present in (ASO, AVSO)	Compound CID: 2116 MF: C₂₉H₅₀O₂ MW: 430.7g/mol InChIKey: GVJHHUAWPYXKBD-UHFFFAOYSA-N IUPAC Name: 2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydrochromen-6-ol Create Date: 2005-03-25
4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- Present in (ASO, AWSO)	Compound CID: 119838 MF: C ₆ H ₈ O ₄ MW: 144.12g/mol InChIKey: VOLMSPGWNYJHQQ-UHFFFAOYSA-N IUPAC Name: 3,5-dihydroxy-6-methyl-2,3-dihdropyran-4-one Create Date: 2005-03-27

Compounds	Chemical (PubChem CID:)	GC MS SPECTRA(Chromatogram)
5-Hydroxymethylfurfural Present in (AWSO)	Compound CID: 237332 MF: C₆H₆O₃ MW: 126.11g/mol InChIKey: NOEGNKMFWQHSLB-UHFFFAOYSA-N IUPAC Name: 5-(hydroxymethyl)furan-2-carbaldehyde Create Date: 2005-03-26
Oleic Acid Present in AWSO, AVSO	Compound CID: 445639 MF: C ₁₈ H ₃₄ O ₂ MW: 282.5g/mol InChIKey: ZQPPMHVWECSIRJ-KTKRTIGZSA-N IUPAC Name: (Z)-octadec-9-enoic acid Create Date: 2004-09-16
.alpha.-D-Glucopyranoside, O-.alpha.-D-glucopyranosyl-(1.fwdarw.3)-.beta.-D-fructofuranosyl Present in AWSO	Compound CID: 220003 MF: C₁₈H₃₂O₁₆ MW: 504.4g/mol InChIKey: QWIZNVHXXZRPDR-UHFFFAOYSA-N IUPAC Name: 2-[4-hydroxy-2,5-bis(hydroxymethyl)-2-[3,4,5-(hydroxymethyl)oxane-3,4,5-triol Create Date: 2005-03-26

Compounds	Chemical (PubChem CID:)	GC MS SPECTRA(Chromatogram)
Palmitic Acid Present in AWSO	Compound CID: 985 MF: C ₁₆ H ₃₂ O ₂ MW: 256.42g/mol InChIKey: IPCSVZSSVZVIGE-UHFFFAOYSA-N IUPAC Name: hexadecanoic acid Create Date: 2004-09-16
Levoglucosenone Present in AWSO	Compound CID: 699486 MF: C₆H₆O₃ MW: 126.11g/mol InChIKey: HITOXZPZGPXYHY-UJURSFKZSA-N IUPAC Name: (1S,5R)-6,8-dioxabicyclo[3.2.1]oct-2-en-4-one Create Date: 2004-09-16
Cyclopropanecarboxylic acid, 3-formyl-2,2-dimethyl-, ethyl ester Present in AWSO	Compound CID: 566079 MF: C ₉ H ₁₄ O ₃ MW: 170.21g/mol InChIKey: ZFZXRNVTYVRULM-UHFFFAOYSA-N IUPAC Name: ethyl 3-formyl-2,2-dimethylcyclopropanecarboxylate Create Date: 2005-03-27
1H-Inden-1-ol, 2,3-dihydro- Present in AWSO	Compound CID: 22819 MF: C ₉ H ₁₀ O MW: 134.17g/mol InChIKey: YIAPLDFPUUJILH-UHFFFAOYSA-N IUPAC Name: 2,3-dihydro-1H-inden-1-ol Create Date: 2004-09-16

Compounds	Chemical (PubChem CID:)	GC MS SPECTRA(Chromatogram)
Phenol, 2,6-bis(1,1-dimethylethyl)- Present in AWSO	Compound CID: 31405 MF: C₁₄H₂₂O MW: 206.32g/mol InChIKey: DKCPKDPYUFEZCP-UHFFFAOYSA-N IUPAC Name: 2,6-ditert-butylphenol Create Date: 2005-03-26
Chloro(2-methyloxiran-2-yl)acetic acid, t-butyl ester Present in AWSO	Compound CID: 545402 MF: C₉H₁₅ClO₃ MW: 206.66g/mol InChIKey: SZVRMPXPAYKBKB-UHFFFAOYSA-N IUPAC Name: tert-butyl 2-chloro-2-(2-methyloxiran-2-yl)acetate Create Date: 2005-03-27
Cyclodecacyclodecene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18-octadecahydro-	Compound CID: 5377998 MF: C ₂₀ H ₃₆ MW: 276.5g/mol InChIKey: YNIDDVZQMSOPPE-VXPUYCOJSA-N IUPAC Name: (1Z)-bicyclo[10.8.0]icos-1(12)-ene Create Date: 2005-03-27

Compounds	Chemical (PubChem CID:)	GC MS SPECTRA(Chromatogram)
2H-Pyran, 2-(7-heptadecynyloxy)tetrahydro-	<p>Compound CID: 543312</p> <p>MF: C₂₂H₄₀O₂</p> <p>MW: 336.6g/mol</p> <p>InChIKey: ONANHJGDQJCYMD-UHFFFAOYSA-N</p> <p>IUPAC Name: 2-heptadec-7-ynoxyoxane</p> <p>Create Date: 2005-03-27</p>
Androstan-17-one, 3-ethyl-3-hydroxy-, (5.alpha.)-	<p>Compound CID: 14681481</p> <p>MF: C₂₁H₃₄O₂</p> <p>MW: 318.5g/mol</p> <p>InChIKey: SPKGPDRGORWGNP-SISSWOJISA-N</p> <p>IUPAC Name: (5S,8R,9S,10S,13S,14S)-3-ethyl-3-hydroxy-10,13-dimethyl-2,4,5,6,7,8,9,11,12,14,15,16-dodecahydro-1H-cyclopenta[a]phenanthren-17-one</p> <p>Create Date: 2007-02-09</p>
Z,E-2,13-Octadecadien-1-ol	<p>Compound CID: 5364462</p> <p>MF: C₁₈H₃₄O</p> <p>MW: 266.5g/mol</p> <p>InChIKey: YCOMGIOWVNOOBC-YZDAJDCNSA-N</p> <p>IUPAC Name: (2Z,13E)-octadeca-2,13-dien-1-ol</p> <p>Create Date: 2005-03-27</p>

Compounds	Chemical (PubChem CID:)	GC MS SPECTRA(Chromatogram)
Chrysene, octadecahydro	<p>Compound CID: 98460</p> <p>MF: C₁₈H₃₀</p> <p>MW: 246.4g/mol</p> <p>InChIKey: ZEMKTMFBYLHVNN-UHFFFAOYSA-N</p> <p>IUPAC Name: 1,2,3,4,4a,4b,5,6,6a,7,8,9,10,10a,10b,11,12,12a-octadecahydrochrysene</p> <p>Create Date: 2005-03-26</p>
Bicyclo[10.6.0]octadeca-1(12),15-diene	<p>Compound CID: 5362802</p> <p>MF: C₁₈H₃₀</p> <p>MW: 246.4g/mol</p> <p>InChIKey: VZCXNHIRQUVFRT-GROAESOISA-N</p> <p>IUPAC Name: (1Z,15Z)-bicyclo[10.6.0]octadeca-1(12),15-diene</p> <p>Create Date: 2005-03-27</p>
3-Chloropropionic acid, heptadecyl ester	<p>Compound CID: 545757</p> <p>MF: C₂₀H₃₉ClO₂</p> <p>MW: 347g/mol</p> <p>InChIKey: UDESWCQJPWPMKY-UHFFFAOYSA-N</p> <p>IUPAC Name: heptadecyl 3-chloropropanoate</p> <p>Create Date: 2005-03-27</p>

Compounds	Chemical (PubChem CID:)	GC MS SPECTRA(Chromatogram)
1-Heptatriacotanol	<p>Compound CID: 537071</p> <p>MF: C₃₇H₇₆O</p> <p>MW: 537g/mol</p> <p>InChIKey: ZGJKNMPTVDDRRH-UHFFFAOYSA-N</p> <p>IUPAC Name: heptatriacontan-1-ol</p> <p>Create Date: 2005-03-27</p>
13-Docosenamide, (Z)-	<p>Compound CID: 5365371</p> <p>MF: C₂₂H₄₃NO</p> <p>MW: 337.6g/mol</p> <p>InChIKey: UAUDZVJPLUQNMU-KTKRTIGZSA-N</p> <p>IUPAC Name: (Z)-docos-13-enamide</p> <p>Create Date: 2005-03-27</p>
Caryophyllene oxide	<p>Compound CID: 1742210</p> <p>MF: C₁₅H₂₄O</p> <p>MW: 220.35g/mol</p> <p>InChIKey: NVEQFIOZRFFVFW-RGCMKSIDSA-N</p> <p>IUPAC Name: (1R,4R,6R,10S)-4,12,12-trimethyl-9-methylidene-5-oxatricyclo[8.2.0.0^{4,6}]dodecane</p> <p>Create Date: 2005-07-12</p>
Heptacosane	<p>Compound CID: 11636</p> <p>MF: C₂₇H₅₆</p> <p>MW: 380.7g/mol</p> <p>InChIKey: BJQWYEJQWHSSCJ-UHFFFAOYSA-N</p> <p>IUPAC Name: heptacosane</p> <p>Create Date: 2004-09-16</p>

Compounds	Chemical (PubChem CID:)	GC MS SPECTRA(Chromatogram)
.gamma.-Tocophero	<p>Compound CID: 91738518</p> <p>MF: C₃₀H₄₇F₃O₃</p> <p>MW: 512.7g/mol</p> <p>InChIKey: OWMUJRCXUOSNAV-UHFFFAOYSA-N</p> <p>IUPAC Name: [2,7,8-trimethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydrochromen-6-yl] 2,2,2-trifluoroacetate</p> <p>Create Date: 2015-04-28</p>
p-Menth-8-en-3-ol, acetate	<p>Compound CID: 94579</p> <p>MF: C₁₂H₂₀O₂</p> <p>MW: 196.29g/mol</p> <p>InChIKey: HLHIVJRL0DSUCI-ADEWGFFLSA-N</p> <p>IUPAC Name: [(1R,2S,5R)-5-methyl-2-prop-1-en-2-ylcyclohexyl] acetate</p> <p>Create Date: 2005-03-26</p>
Scarlal (sclareolide lactol)	<p>Compound CID: 537618</p> <p>MF: C₁₆H₂₈O₂</p> <p>MW: 252.39g/mol</p> <p>InChIKey: UZSSRRVZGDVPRE-UHFFFAOYSA-N</p> <p>IUPAC Name: 3a,6,6,9a-tetramethyl-2,4,5,5a,7,8,9,9b-octahydro-1H-benzo[e][1]benzofuran-2-ol</p> <p>Create Date: 2005-03-27</p>

Compounds	Chemical (PubChem CID:)	GC MS SPECTRA(Chromatogram)
12-Methyl-E,E-2,13-octadecadien-1-ol	<p>Compound CID: 90107969</p> <p>MF: C₁₉H₃₆O</p> <p>MW: 280.5g/mol</p> <p>InChIKey: QQRKGLQLQDQGGI-WSGPNKEYSA-N</p> <p>IUPAC Name: (2E,13E)-12-methyloctadeca-2,13-dien-1-ol</p> <p>Create Date: 2015-02-13</p>
Phenol, 2,5-bis(1,1-dimethylethyl)-	<p>Compound CID: 79983</p> <p>MF: C₁₄H₂₂O</p> <p>MW: 206.32g/mol</p> <p>InChIKey: KDBZVULQVCUNNA-UHFFFAOYSA-N</p> <p>IUPAC Name: 2,5-ditert-butylphenol</p> <p>Create Date: 2005-03-26</p>
2-Acetoxy-1,1,10-trimethyl-6,9-epidioxycyclohexyl	<p>Compound CID: 538309</p> <p>MF: C₁₅H₂₄O₄</p> <p>MW: 268.35g/mol</p> <p>InChIKey: GNQFBOZHHSYHCB-UHFFFAOYSA-N</p> <p>IUPAC Name: (2,2,6-trimethyl-9,10-dioxatricyclo[6.2.2.0^{1,6}]dodecan-3-yl) acetate</p> <p>Create Date: 2005-03-27</p>

Compounds	Chemical (PubChem CID:)	GC MS SPECTRA(Chromatogram)
3H-3,10a-Methano-1,2-benzodioxocin-3-ol, octahydro-7,7-dimethyl-, (3.alpha.,6a.beta.,10a.beta.)-	<p>Compound CID: 606210</p> <p>MF: C₁₃H₂₂O₃</p> <p>MW: 226.31g/mol</p> <p>InChIKey: RBFWHMUVCHUYON-UHFFFAOYSA-N</p> <p>IUPAC Name: 5,5-dimethyl-11,12-dioxatricyclo[8.2.1.01,6]tridecan-10-ol</p> <p>Create Date: 2005-03-27</p>
Tricyclo[4.3.0.0(7,9)]nonane, 2,2,5,5,8,8-hexamethyl-, (1.alpha.,6.beta.,7.alpha.,9.alpha.)-	<p>Compound CID: 549738</p> <p>MF: C₁₅H₂₆</p> <p>MW: 206.37g/mol</p> <p>InChIKey: PUJIBQKSZBPAMT-UHFFFAOYSA-N</p> <p>IUPAC Name: 2,2,5,5,8,8-hexamethyltricyclo[4.3.0.07,9]nonane</p> <p>Create Date: 2005-03-27</p>
GSO: Grape (Vitis vinifera) extracts; PSO: Plum (Prunus subg. Prunus: Mirabelles) extracts; ASO: Apple (Malus domestic) extracts; AWSO: Ajwa dates (Phoenix dactylifera L) extracts; PGSO: Pomegranate (Punica granatum) extracts; AVSO: Avocado (Persea Americana) extracts.		

Table 7: Results of the GC-MS chromatogram of the selected compounds in studied seeds (GSO, PSO, ASO, AWSO, PGSO and AVSO).

Docking Protein (Epinephrine Receptor PDB: 2rh1) with the Ligand (Seeds GSO, PSO, ASO, AWSO, PGSO and AVSO) Phytochemical Molecule and the ACE2 Receptor

The epinephrine receptor PDB: 2rh1 and ACE2 receptor 3D0G (Table 8) showed binding energy with the six studied seeds in the current study's oils extracts 44 ligands (Table 9). Table 9 reflects the binding affinity of 44 ligands to both investigated receptors. These docking studies showed that among the seed extract phytochemicals, the stigmastan-3,5-diene (compound CID: 525918, MF: C₂₉H₄₈) component of GSO, PSO, AWSO, PGSO and AVSO had the highest binding affinity of -11.4 kcal/mole and -11.6 kcal/mole, with 2rh1 and 3D0G,

respectively. Moreover, the levoglucosenone (compound CID: 699486, MF: C₆H₆O₃) component of AWSO extract had the lowest binding affinity at -4.8 kcal/mole and 5.5 kcal/mole with 2rh1 and 3D0G, respectively, as given in Table 10. The ligands with the best possible affinity to the receptor 2rh1 and ACE2 receptor 3D0G are outlined in Table 10, while the comparison of the highest binding energy is provided in Fig. 2.

Figure 2: Comparison between the highest binding affinity (kcal/mole) interaction of 44 ligands of GSO, PSO, ASO, AWSO, PGSO and AVSO with the β 2 adrenoreceptor (2rh1) and ACE2 receptor (3D0G) in the AutoDock analysis. (GSO: Grapes (*Vitis vinifera*) extracts; PSO: Plum (*Prunus* subg. *Prunus*: *Mirabelles*) extracts; ASO: Apple (*Malus domestica*) extracts; AWSO: Ajwa dates (*Phoenix dactylifera* L) extracts; PGSO: Pomegranate (*Punica granatum*) extracts; AVSO: Avocado (*Persea Americana*) extracts).

Target	Target protein receptor (PDB)
1-Epinephrine (adrenaline) To potential antistress	<p>β2 adrenoreceptor (PDB: 2rh1)</p> <ul style="list-style-type: none"> High-resolution crystal structure of human B2-adrenergic G protein-coupled receptor DOI: 10.2210/pdb2RH1/pdb Classification: MEMBRANE PROTEIN/HYDROLASE Organism(s): Homo sapiens, Escherichia virus T4

	<ul style="list-style-type: none"> • Expression system: Spodoptera frugiperda <p>3D structure of 2rh1</p> <p>Deposition author(s): Cherezov, V., Rosenbaum, D.M., Hanson, M.A., Rasmussen, S.G.F., Thian, F.S., Kobilka, T.S., Choi, H.J., Kuhn, P., Weis, W.I., Kobilka, B.K., Stevens, R.C., Accelerated Technologies Center for Gene to 3D Structure (ATCG3D), GPCR Network (GPCR).</p>
<p>2-Angiotensin-converting enzyme 2 The ACE2 receptor</p> <p>The SARS-CoV-2 virus requires ACE2 to infect cells</p> <p>to potential new clinical trial tests ACE inhibitor against SARS-CoV-2</p>	<p>3D0G</p> <ul style="list-style-type: none"> • Crystal structure of spike protein receptor-binding domain from the 2002-2003 SARS coronavirus human strain complexed with human-civet chimeric receptor ACE2 • -DOI: 10.2210/pdb3D0G/pdb • -Classification: HYDROLASE • -Organism(s): Paguma larvata, Homo sapiens, Severe acute respiratory syndrome-related coronavirus • -Expression System: Spodoptera frugiperda • -Mutation(s): No • -Deposited: 2008-05-01 Released: 2008-07-08 <p>-Deposition Author(s): Li, F.</p> <p>3D structure of 3D0G</p>

Table 8: The target receptors used in AutoDock analysis.

Compounds separated by GC-MS	Chemical (PubChem CID:)	AutoDock analysis results with 2rh1	AutoDock analysis results with 3D0G																																																																																
9-Octadecenamide, (Z)- Or Oleamide Present in all(GSO, PSO, ASO, AWSO, PGSO, AVSO)	Compound CID: 5283387	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-7.9</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-7.6</td><td>18.099</td><td>20.258</td></tr> <tr><td>3</td><td>-7.5</td><td>4.936</td><td>6.041</td></tr> <tr><td>4</td><td>-7.5</td><td>16.137</td><td>18.106</td></tr> <tr><td>5</td><td>-7.3</td><td>15.746</td><td>17.992</td></tr> <tr><td>6</td><td>-7.3</td><td>5.597</td><td>7.999</td></tr> <tr><td>7</td><td>-7.2</td><td>18.880</td><td>21.213</td></tr> <tr><td>8</td><td>-7.2</td><td>15.609</td><td>17.691</td></tr> <tr><td>9</td><td>-7.2</td><td>3.937</td><td>5.666</td></tr> </table>	mode	affinity (kcal/mol)	dist from rmsd l.b.	best mode rmsd u.b.	1	-7.9	0.000	0.000	2	-7.6	18.099	20.258	3	-7.5	4.936	6.041	4	-7.5	16.137	18.106	5	-7.3	15.746	17.992	6	-7.3	5.597	7.999	7	-7.2	18.880	21.213	8	-7.2	15.609	17.691	9	-7.2	3.937	5.666	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-8.7</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-7.9</td><td>20.179</td><td>23.329</td></tr> <tr><td>3</td><td>-7.9</td><td>5.328</td><td>7.631</td></tr> <tr><td>4</td><td>-7.9</td><td>3.152</td><td>6.182</td></tr> <tr><td>5</td><td>-7.4</td><td>12.064</td><td>14.571</td></tr> <tr><td>6</td><td>-7.2</td><td>38.123</td><td>41.406</td></tr> <tr><td>7</td><td>-7.2</td><td>11.796</td><td>15.162</td></tr> <tr><td>8</td><td>-7.1</td><td>37.831</td><td>41.165</td></tr> <tr><td>9</td><td>-6.9</td><td>22.241</td><td>24.735</td></tr> </table>	mode	affinity (kcal/mol)	dist from rmsd l.b.	best mode rmsd u.b.	1	-8.7	0.000	0.000	2	-7.9	20.179	23.329	3	-7.9	5.328	7.631	4	-7.9	3.152	6.182	5	-7.4	12.064	14.571	6	-7.2	38.123	41.406	7	-7.2	11.796	15.162	8	-7.1	37.831	41.165	9	-6.9	22.241	24.735
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Stigmastan-3,5-diene Present in (GSO, PSO, AWSO, PGSO, AVSO)	Compound CID: 525918	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-11.4</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-11.3</td><td>0.585</td><td>1.270</td></tr> <tr><td>3</td><td>-11.2</td><td>0.859</td><td>1.524</td></tr> <tr><td>4</td><td>-10.6</td><td>0.745</td><td>6.388</td></tr> <tr><td>5</td><td>-10.5</td><td>3.520</td><td>6.120</td></tr> <tr><td>6</td><td>-10.5</td><td>15.179</td><td>17.760</td></tr> <tr><td>7</td><td>-10.5</td><td>15.145</td><td>17.803</td></tr> <tr><td>8</td><td>-10.4</td><td>15.267</td><td>16.785</td></tr> <tr><td>9</td><td>-10.3</td><td>17.747</td><td>19.766</td></tr> </table>	mode	affinity (kcal/mol)	dist from rmsd l.b.	best mode rmsd u.b.	1	-11.4	0.000	0.000	2	-11.3	0.585	1.270	3	-11.2	0.859	1.524	4	-10.6	0.745	6.388	5	-10.5	3.520	6.120	6	-10.5	15.179	17.760	7	-10.5	15.145	17.803	8	-10.4	15.267	16.785	9	-10.3	17.747	19.766	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-11.6</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-10.9</td><td>1.283</td><td>2.433</td></tr> <tr><td>3</td><td>-10.9</td><td>39.727</td><td>42.068</td></tr> <tr><td>4</td><td>-10.7</td><td>39.780</td><td>42.129</td></tr> <tr><td>5</td><td>-10.4</td><td>39.824</td><td>42.157</td></tr> <tr><td>6</td><td>-10.3</td><td>3.741</td><td>7.079</td></tr> <tr><td>7</td><td>-10.1</td><td>39.787</td><td>42.098</td></tr> <tr><td>8</td><td>-9.9</td><td>40.043</td><td>42.330</td></tr> <tr><td>9</td><td>-9.9</td><td>1.193</td><td>1.984</td></tr> </table>	mode	affinity (kcal/mol)	dist from rmsd l.b.	best mode rmsd u.b.	1	-11.6	0.000	0.000	2	-10.9	1.283	2.433	3	-10.9	39.727	42.068	4	-10.7	39.780	42.129	5	-10.4	39.824	42.157	6	-10.3	3.741	7.079	7	-10.1	39.787	42.098	8	-9.9	40.043	42.330	9	-9.9	1.193	1.984
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Hexadecanamide Present in all(GSO, PSO, ASO, AWSO, PGSO, AVSO)	Compound CID: 69421	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-6.6</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.5</td><td>3.001</td><td>3.063</td></tr> <tr><td>3</td><td>-6.5</td><td>28.774</td><td>29.830</td></tr> <tr><td>4</td><td>-6.5</td><td>5.034</td><td>8.653</td></tr> <tr><td>5</td><td>-6.4</td><td>4.445</td><td>8.659</td></tr> <tr><td>6</td><td>-6.4</td><td>28.657</td><td>28.936</td></tr> <tr><td>7</td><td>-6.3</td><td>16.919</td><td>17.687</td></tr> <tr><td>8</td><td>-6.2</td><td>5.533</td><td>8.943</td></tr> <tr><td>9</td><td>-6.1</td><td>17.367</td><td>19.129</td></tr> </table>	mode	affinity (kcal/mol)	dist from rmsd l.b.	best mode rmsd u.b.	1	-6.6	0.000	0.000	2	-6.5	3.001	3.063	3	-6.5	28.774	29.830	4	-6.5	5.034	8.653	5	-6.4	4.445	8.659	6	-6.4	28.657	28.936	7	-6.3	16.919	17.687	8	-6.2	5.533	8.943	9	-6.1	17.367	19.129	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-7.7</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-7.3</td><td>4.351</td><td>8.455</td></tr> <tr><td>3</td><td>-6.5</td><td>3.234</td><td>4.260</td></tr> <tr><td>4</td><td>-6.5</td><td>41.198</td><td>42.804</td></tr> <tr><td>5</td><td>-6.4</td><td>39.960</td><td>41.558</td></tr> <tr><td>6</td><td>-6.4</td><td>41.356</td><td>42.885</td></tr> <tr><td>7</td><td>-6.2</td><td>14.612</td><td>16.312</td></tr> <tr><td>8</td><td>-6.1</td><td>36.548</td><td>38.880</td></tr> <tr><td>9</td><td>-6.1</td><td>0.874</td><td>1.773</td></tr> </table>	mode	affinity (kcal/mol)	dist from rmsd l.b.	best mode rmsd u.b.	1	-7.7	0.000	0.000	2	-7.3	4.351	8.455	3	-6.5	3.234	4.260	4	-6.5	41.198	42.804	5	-6.4	39.960	41.558	6	-6.4	41.356	42.885	7	-6.2	14.612	16.312	8	-6.1	36.548	38.880	9	-6.1	0.874	1.773
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Pentanoic acid, 5-hydroxy-, 2,4-di-t-butylphenyl esters Present in GSO, PSO , PGSO	Compound CID: 605777	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-10.2</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-9.1</td><td>2.389</td><td>4.585</td></tr> <tr><td>3</td><td>-9.0</td><td>2.106</td><td>5.787</td></tr> <tr><td>4</td><td>-9.0</td><td>1.775</td><td>2.116</td></tr> <tr><td>5</td><td>-8.8</td><td>3.946</td><td>4.997</td></tr> <tr><td>6</td><td>-8.8</td><td>17.782</td><td>19.552</td></tr> <tr><td>7</td><td>-8.7</td><td>3.147</td><td>4.417</td></tr> <tr><td>8</td><td>-8.6</td><td>2.895</td><td>5.850</td></tr> <tr><td>9</td><td>-8.4</td><td>17.459</td><td>19.674</td></tr> </table>	mode	affinity (kcal/mol)	dist from rmsd l.b.	best mode rmsd u.b.	1	-10.2	0.000	0.000	2	-9.1	2.389	4.585	3	-9.0	2.106	5.787	4	-9.0	1.775	2.116	5	-8.8	3.946	4.997	6	-8.8	17.782	19.552	7	-8.7	3.147	4.417	8	-8.6	2.895	5.850	9	-8.4	17.459	19.674	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-10.1</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-9.6</td><td>2.022</td><td>3.395</td></tr> <tr><td>3</td><td>-8.6</td><td>1.230</td><td>2.714</td></tr> <tr><td>4</td><td>-8.3</td><td>2.533</td><td>4.800</td></tr> <tr><td>5</td><td>-8.2</td><td>22.549</td><td>24.947</td></tr> <tr><td>6</td><td>-7.9</td><td>19.527</td><td>21.457</td></tr> <tr><td>7</td><td>-7.9</td><td>17.847</td><td>20.003</td></tr> <tr><td>8</td><td>-7.8</td><td>2.135</td><td>5.492</td></tr> <tr><td>9</td><td>-7.7</td><td>12.176</td><td>14.396</td></tr> </table>	mode	affinity (kcal/mol)	dist from rmsd l.b.	best mode rmsd u.b.	1	-10.1	0.000	0.000	2	-9.6	2.022	3.395	3	-8.6	1.230	2.714	4	-8.3	2.533	4.800	5	-8.2	22.549	24.947	6	-7.9	19.527	21.457	7	-7.9	17.847	20.003	8	-7.8	2.135	5.492	9	-7.7	12.176	14.396
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1	-5.7	0.000	0.000																																																																																
2	-5.7	42.507	44.325																																																																																
3	-5.5	4.481	7.289																																																																																
4	-5.4	41.300	43.326																																																																																
5	-5.3	37.851	40.664																																																																																
6	-5.3	25.680	26.555																																																																																
7	-5.1	15.442	17.774																																																																																
8	-5.1	14.625	19.346																																																																																
9	-5.0	4.282	9.634																																																																																
1,3-Benzenediol, o-(4-methylbenzoyl)-o'-(2-methoxybenzoyl)- Present in GSO, PSO, ONLY	Compound CID: 91715040	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-10.3</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-10.2</td><td>0.675</td><td>5.542</td></tr> <tr><td>3</td><td>-9.6</td><td>2.910</td><td>4.643</td></tr> <tr><td>4</td><td>-9.5</td><td>1.981</td><td>5.697</td></tr> <tr><td>5</td><td>-9.5</td><td>2.724</td><td>5.991</td></tr> <tr><td>6</td><td>-9.4</td><td>2.390</td><td>5.481</td></tr> <tr><td>7</td><td>-9.3</td><td>1.847</td><td>2.692</td></tr> <tr><td>8</td><td>-9.2</td><td>3.100</td><td>4.553</td></tr> <tr><td>9</td><td>-9.2</td><td>2.602</td><td>5.707</td></tr> </table>	mode	affinity (kcal/mol)	dist from rmsd l.b.	best mode rmsd u.b.	1	-10.3	0.000	0.000	2	-10.2	0.675	5.542	3	-9.6	2.910	4.643	4	-9.5	1.981	5.697	5	-9.5	2.724	5.991	6	-9.4	2.390	5.481	7	-9.3	1.847	2.692	8	-9.2	3.100	4.553	9	-9.2	2.602	5.707	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-9.5</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-9.5</td><td>40.358</td><td>41.887</td></tr> <tr><td>3</td><td>-9.4</td><td>40.341</td><td>41.920</td></tr> <tr><td>4</td><td>-9.3</td><td>3.011</td><td>4.294</td></tr> <tr><td>5</td><td>-9.0</td><td>41.368</td><td>42.932</td></tr> <tr><td>6</td><td>-8.9</td><td>2.298</td><td>4.249</td></tr> <tr><td>7</td><td>-8.8</td><td>1.507</td><td>2.187</td></tr> <tr><td>8</td><td>-8.4</td><td>23.006</td><td>25.172</td></tr> <tr><td>9</td><td>-8.4</td><td>40.941</td><td>42.410</td></tr> </table>	mode	affinity (kcal/mol)	dist from rmsd l.b.	best mode rmsd u.b.	1	-9.5	0.000	0.000	2	-9.5	40.358	41.887	3	-9.4	40.341	41.920	4	-9.3	3.011	4.294	5	-9.0	41.368	42.932	6	-8.9	2.298	4.249	7	-8.8	1.507	2.187	8	-8.4	23.006	25.172	9	-8.4	40.941	42.410
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Compounds separated by GC-MS	Chemical (PubChem CID:)	AutoDock analysis results with 2rh1	AutoDock analysis results with 3D0G																																																																																
2-Bromotetradecane GSO, AVSO ONLY	Compound CID: 12798926	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-5.4</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-5.4</td><td>15.158</td><td>16.890</td></tr> <tr><td>3</td><td>-5.4</td><td>1.113</td><td>2.254</td></tr> <tr><td>4</td><td>-5.3</td><td>1.468</td><td>2.327</td></tr> <tr><td>5</td><td>-5.2</td><td>10.124</td><td>10.524</td></tr> <tr><td>6</td><td>-5.1</td><td>2.373</td><td>5.986</td></tr> <tr><td>7</td><td>-5.1</td><td>29.072</td><td>29.833</td></tr> <tr><td>8</td><td>-5.1</td><td>14.628</td><td>15.594</td></tr> <tr><td>9</td><td>-4.8</td><td>18.639</td><td>19.593</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-5.4	0.000	0.000	2	-5.4	15.158	16.890	3	-5.4	1.113	2.254	4	-5.3	1.468	2.327	5	-5.2	10.124	10.524	6	-5.1	2.373	5.986	7	-5.1	29.072	29.833	8	-5.1	14.628	15.594	9	-4.8	18.639	19.593	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-6.1</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.0</td><td>2.108</td><td>2.892</td></tr> <tr><td>3</td><td>-5.7</td><td>2.869</td><td>6.951</td></tr> <tr><td>4</td><td>-5.4</td><td>3.121</td><td>6.816</td></tr> <tr><td>5</td><td>-5.3</td><td>3.101</td><td>7.078</td></tr> <tr><td>6</td><td>-5.1</td><td>39.205</td><td>41.147</td></tr> <tr><td>7</td><td>-5.0</td><td>1.008</td><td>2.018</td></tr> <tr><td>8</td><td>-4.9</td><td>2.696</td><td>5.165</td></tr> <tr><td>9</td><td>-4.8</td><td>4.346</td><td>4.954</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-6.1	0.000	0.000	2	-6.0	2.108	2.892	3	-5.7	2.869	6.951	4	-5.4	3.121	6.816	5	-5.3	3.101	7.078	6	-5.1	39.205	41.147	7	-5.0	1.008	2.018	8	-4.9	2.696	5.165	9	-4.8	4.346	4.954
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Isooctyl 3-mercaptopropionate GSO ONLY	Compound CID: 104386	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-6.4</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.3</td><td>14.765</td><td>16.077</td></tr> <tr><td>3</td><td>-6.2</td><td>11.667</td><td>12.163</td></tr> <tr><td>4</td><td>-6.2</td><td>17.823</td><td>19.080</td></tr> <tr><td>5</td><td>-5.9</td><td>8.329</td><td>8.726</td></tr> <tr><td>6</td><td>-5.7</td><td>29.031</td><td>29.914</td></tr> <tr><td>7</td><td>-5.5</td><td>13.740</td><td>14.480</td></tr> <tr><td>8</td><td>-5.5</td><td>16.863</td><td>17.844</td></tr> <tr><td>9</td><td>-5.4</td><td>2.400</td><td>3.828</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-6.4	0.000	0.000	2	-6.3	14.765	16.077	3	-6.2	11.667	12.163	4	-6.2	17.823	19.080	5	-5.9	8.329	8.726	6	-5.7	29.031	29.914	7	-5.5	13.740	14.480	8	-5.5	16.863	17.844	9	-5.4	2.400	3.828	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-7.2</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.5</td><td>39.208</td><td>40.341</td></tr> <tr><td>3</td><td>-6.3</td><td>2.006</td><td>2.363</td></tr> <tr><td>4</td><td>-5.9</td><td>4.793</td><td>5.592</td></tr> <tr><td>5</td><td>-5.9</td><td>42.500</td><td>43.305</td></tr> <tr><td>6</td><td>-5.8</td><td>4.040</td><td>4.380</td></tr> <tr><td>7</td><td>-5.7</td><td>12.606</td><td>14.585</td></tr> <tr><td>8</td><td>-5.7</td><td>35.877</td><td>37.482</td></tr> <tr><td>9</td><td>-5.6</td><td>22.500</td><td>23.514</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-7.2	0.000	0.000	2	-6.5	39.208	40.341	3	-6.3	2.006	2.363	4	-5.9	4.793	5.592	5	-5.9	42.500	43.305	6	-5.8	4.040	4.380	7	-5.7	12.606	14.585	8	-5.7	35.877	37.482	9	-5.6	22.500	23.514
mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.																																																																																
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Squalene Present in(PSO, ASO, AWSO, PGSO, AVSO	Compound CID: 638072	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-10.6</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-10.4</td><td>20.457</td><td>24.866</td></tr> <tr><td>3</td><td>-10.3</td><td>17.188</td><td>21.755</td></tr> <tr><td>4</td><td>-10.1</td><td>1.067</td><td>11.706</td></tr> <tr><td>5</td><td>-10.1</td><td>17.567</td><td>19.553</td></tr> <tr><td>6</td><td>-9.9</td><td>16.453</td><td>17.878</td></tr> <tr><td>7</td><td>-9.7</td><td>20.700</td><td>24.348</td></tr> <tr><td>8</td><td>-9.4</td><td>2.646</td><td>3.277</td></tr> <tr><td>9</td><td>-9.1</td><td>15.534</td><td>17.685</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-10.6	0.000	0.000	2	-10.4	20.457	24.866	3	-10.3	17.188	21.755	4	-10.1	1.067	11.706	5	-10.1	17.567	19.553	6	-9.9	16.453	17.878	7	-9.7	20.700	24.348	8	-9.4	2.646	3.277	9	-9.1	15.534	17.685	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-9.7</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-9.2</td><td>16.231</td><td>22.182</td></tr> <tr><td>3</td><td>-9.1</td><td>1.199</td><td>2.245</td></tr> <tr><td>4</td><td>-9.1</td><td>16.484</td><td>23.423</td></tr> <tr><td>5</td><td>-9.0</td><td>15.253</td><td>18.738</td></tr> <tr><td>6</td><td>-8.9</td><td>7.835</td><td>11.977</td></tr> <tr><td>7</td><td>-8.9</td><td>16.454</td><td>22.549</td></tr> <tr><td>8</td><td>-8.8</td><td>1.351</td><td>3.257</td></tr> <tr><td>9</td><td>-8.8</td><td>16.602</td><td>18.249</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-9.7	0.000	0.000	2	-9.2	16.231	22.182	3	-9.1	1.199	2.245	4	-9.1	16.484	23.423	5	-9.0	15.253	18.738	6	-8.9	7.835	11.977	7	-8.9	16.454	22.549	8	-8.8	1.351	3.257	9	-8.8	16.602	18.249
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2	-6.4	17.058	18.805																																																																																
3	-6.4	19.059	20.581																																																																																
4	-6.4	15.611	17.024																																																																																
5	-6.3	16.676	18.455																																																																																
6	-6.3	16.057	16.676																																																																																
7	-6.3	5.952	8.589																																																																																
8	-6.1	16.320	18.295																																																																																
9	-6.1	19.622	21.090																																																																																
mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.																																																																																
1	-6.5	0.000	0.000																																																																																
2	-6.4	2.004	2.058																																																																																
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4	-5.7	14.643	17.558																																																																																
5	-5.6	3.983	8.217																																																																																
6	-5.5	37.549	40.072																																																																																
7	-5.4	26.598	27.120																																																																																
8	-5.4	36.672	38.758																																																																																
9	-5.4	23.623	24.270																																																																																
1,2-15,16-Diepoxyhexadecane	Compound CID: 543423	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-5.8</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-5.7</td><td>9.725</td><td>9.966</td></tr> <tr><td>3</td><td>-5.7</td><td>9.858</td><td>10.153</td></tr> <tr><td>4</td><td>-5.6</td><td>18.378</td><td>20.441</td></tr> <tr><td>5</td><td>-5.5</td><td>10.388</td><td>12.939</td></tr> <tr><td>6</td><td>-5.4</td><td>17.847</td><td>19.675</td></tr> <tr><td>7</td><td>-5.4</td><td>31.635</td><td>32.652</td></tr> <tr><td>8</td><td>-5.4</td><td>32.480</td><td>33.643</td></tr> <tr><td>9</td><td>-5.3</td><td>10.207</td><td>11.959</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-5.8	0.000	0.000	2	-5.7	9.725	9.966	3	-5.7	9.858	10.153	4	-5.6	18.378	20.441	5	-5.5	10.388	12.939	6	-5.4	17.847	19.675	7	-5.4	31.635	32.652	8	-5.4	32.480	33.643	9	-5.3	10.207	11.959	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-6.3</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.2</td><td>39.652</td><td>41.683</td></tr> <tr><td>3</td><td>-6.1</td><td>40.259</td><td>41.352</td></tr> <tr><td>4</td><td>-5.8</td><td>20.013</td><td>22.417</td></tr> <tr><td>5</td><td>-5.7</td><td>20.848</td><td>21.550</td></tr> <tr><td>6</td><td>-5.5</td><td>19.621</td><td>23.813</td></tr> <tr><td>7</td><td>-5.4</td><td>21.163</td><td>22.331</td></tr> <tr><td>8</td><td>-5.4</td><td>2.897</td><td>8.473</td></tr> <tr><td>9</td><td>-5.1</td><td>33.823</td><td>36.719</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-6.3	0.000	0.000	2	-6.2	39.652	41.683	3	-6.1	40.259	41.352	4	-5.8	20.013	22.417	5	-5.7	20.848	21.550	6	-5.5	19.621	23.813	7	-5.4	21.163	22.331	8	-5.4	2.897	8.473	9	-5.1	33.823	36.719
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cis-Vaccenic acid ASO ONLY	Compound CID: 5282761	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-8.2</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-8.0</td><td>2.390</td><td>3.617</td></tr> <tr><td>3</td><td>-7.9</td><td>4.257</td><td>8.694</td></tr> <tr><td>4</td><td>-7.8</td><td>4.674</td><td>8.707</td></tr> <tr><td>5</td><td>-7.8</td><td>3.732</td><td>5.420</td></tr> <tr><td>6</td><td>-7.7</td><td>16.328</td><td>19.254</td></tr> <tr><td>7</td><td>-7.6</td><td>14.872</td><td>16.498</td></tr> <tr><td>8</td><td>-7.5</td><td>4.960</td><td>7.120</td></tr> <tr><td>9</td><td>-7.2</td><td>9.652</td><td>11.887</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-8.2	0.000	0.000	2	-8.0	2.390	3.617	3	-7.9	4.257	8.694	4	-7.8	4.674	8.707	5	-7.8	3.732	5.420	6	-7.7	16.328	19.254	7	-7.6	14.872	16.498	8	-7.5	4.960	7.120	9	-7.2	9.652	11.887	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-9.3</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-7.9</td><td>2.914</td><td>5.026</td></tr> <tr><td>3</td><td>-7.7</td><td>5.273</td><td>7.773</td></tr> <tr><td>4</td><td>-7.7</td><td>2.736</td><td>5.919</td></tr> <tr><td>5</td><td>-7.4</td><td>36.787</td><td>39.883</td></tr> <tr><td>6</td><td>-7.3</td><td>37.079</td><td>40.202</td></tr> <tr><td>7</td><td>-7.2</td><td>20.426</td><td>23.549</td></tr> <tr><td>8</td><td>-7.2</td><td>21.891</td><td>25.323</td></tr> <tr><td>9</td><td>-7.1</td><td>10.845</td><td>13.308</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-9.3	0.000	0.000	2	-7.9	2.914	5.026	3	-7.7	5.273	7.773	4	-7.7	2.736	5.919	5	-7.4	36.787	39.883	6	-7.3	37.079	40.202	7	-7.2	20.426	23.549	8	-7.2	21.891	25.323	9	-7.1	10.845	13.308
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Compounds separated by GC-MS	Chemical (PubChem CID:)	AutoDock analysis results with 2rh1	AutoDock analysis results with 3D0G																																																																																
cis-11-Eicosenamide Present in (ASO, AWSO, PGSO, AVSO)	Compound CID: 5365374	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-7.5</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-7.3</td><td>18.006</td><td>19.740</td></tr> <tr><td>3</td><td>-7.3</td><td>18.110</td><td>20.418</td></tr> <tr><td>4</td><td>-7.3</td><td>18.155</td><td>20.562</td></tr> <tr><td>5</td><td>-7.3</td><td>18.241</td><td>20.308</td></tr> <tr><td>6</td><td>-7.3</td><td>18.089</td><td>20.815</td></tr> <tr><td>7</td><td>-7.2</td><td>5.373</td><td>7.642</td></tr> <tr><td>8</td><td>-7.2</td><td>5.747</td><td>8.050</td></tr> <tr><td>9</td><td>-7.2</td><td>18.630</td><td>22.568</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-7.5	0.000	0.000	2	-7.3	18.006	19.740	3	-7.3	18.110	20.418	4	-7.3	18.155	20.562	5	-7.3	18.241	20.308	6	-7.3	18.089	20.815	7	-7.2	5.373	7.642	8	-7.2	5.747	8.050	9	-7.2	18.630	22.568	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-7.5</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-7.4</td><td>3.668</td><td>6.248</td></tr> <tr><td>3</td><td>-7.1</td><td>41.086</td><td>43.311</td></tr> <tr><td>4</td><td>-7.0</td><td>4.843</td><td>9.719</td></tr> <tr><td>5</td><td>-6.9</td><td>41.469</td><td>43.778</td></tr> <tr><td>6</td><td>-6.8</td><td>40.595</td><td>42.788</td></tr> <tr><td>7</td><td>-6.8</td><td>14.679</td><td>17.451</td></tr> <tr><td>8</td><td>-6.8</td><td>23.576</td><td>24.796</td></tr> <tr><td>9</td><td>-6.8</td><td>16.583</td><td>20.784</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-7.5	0.000	0.000	2	-7.4	3.668	6.248	3	-7.1	41.086	43.311	4	-7.0	4.843	9.719	5	-6.9	41.469	43.778	6	-6.8	40.595	42.788	7	-6.8	14.679	17.451	8	-6.8	23.576	24.796	9	-6.8	16.583	20.784
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2-Furancarboxaldehyde, 5-methyl- Present in (ASO)only	Compound CID: 12097	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-5.2</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-4.9</td><td>1.129</td><td>2.706</td></tr> <tr><td>3</td><td>-4.7</td><td>13.727</td><td>14.148</td></tr> <tr><td>4</td><td>-4.5</td><td>16.486</td><td>17.349</td></tr> <tr><td>5</td><td>-4.4</td><td>16.326</td><td>17.340</td></tr> <tr><td>6</td><td>-4.4</td><td>25.776</td><td>27.144</td></tr> <tr><td>7</td><td>-4.4</td><td>13.807</td><td>14.344</td></tr> <tr><td>8</td><td>-4.3</td><td>13.371</td><td>13.914</td></tr> <tr><td>9</td><td>-4.1</td><td>13.784</td><td>14.024</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-5.2	0.000	0.000	2	-4.9	1.129	2.706	3	-4.7	13.727	14.148	4	-4.5	16.486	17.349	5	-4.4	16.326	17.340	6	-4.4	25.776	27.144	7	-4.4	13.807	14.344	8	-4.3	13.371	13.914	9	-4.1	13.784	14.024	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-5.5</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-5.5</td><td>1.297</td><td>2.670</td></tr> <tr><td>3</td><td>-5.0</td><td>26.503</td><td>27.470</td></tr> <tr><td>4</td><td>-5.0</td><td>27.596</td><td>28.509</td></tr> <tr><td>5</td><td>-4.8</td><td>27.405</td><td>28.362</td></tr> <tr><td>6</td><td>-4.7</td><td>27.262</td><td>28.243</td></tr> <tr><td>7</td><td>-4.7</td><td>38.756</td><td>39.648</td></tr> <tr><td>8</td><td>-4.7</td><td>36.701</td><td>37.628</td></tr> <tr><td>9</td><td>-4.6</td><td>27.992</td><td>28.935</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-5.5	0.000	0.000	2	-5.5	1.297	2.670	3	-5.0	26.503	27.470	4	-5.0	27.596	28.509	5	-4.8	27.405	28.362	6	-4.7	27.262	28.243	7	-4.7	38.756	39.648	8	-4.7	36.701	37.628	9	-4.6	27.992	28.935
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dl-.alpha.-Tocopherol Present in (ASO, AVSO)	Compound CID: 2116	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-10.2</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-10.0</td><td>2.757</td><td>9.686</td></tr> <tr><td>3</td><td>-9.8</td><td>1.340</td><td>2.205</td></tr> <tr><td>4</td><td>-9.8</td><td>16.886</td><td>18.784</td></tr> <tr><td>5</td><td>-9.5</td><td>17.389</td><td>20.425</td></tr> <tr><td>6</td><td>-9.3</td><td>2.438</td><td>9.526</td></tr> <tr><td>7</td><td>-9.3</td><td>16.900</td><td>18.744</td></tr> <tr><td>8</td><td>-9.2</td><td>27.929</td><td>29.786</td></tr> <tr><td>9</td><td>-9.2</td><td>21.710</td><td>23.493</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-10.2	0.000	0.000	2	-10.0	2.757	9.686	3	-9.8	1.340	2.205	4	-9.8	16.886	18.784	5	-9.5	17.389	20.425	6	-9.3	2.438	9.526	7	-9.3	16.900	18.744	8	-9.2	27.929	29.786	9	-9.2	21.710	23.493	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-9.2</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-9.1</td><td>2.644</td><td>9.430</td></tr> <tr><td>3</td><td>-9.0</td><td>15.398</td><td>17.005</td></tr> <tr><td>4</td><td>-8.9</td><td>24.686</td><td>27.320</td></tr> <tr><td>5</td><td>-8.5</td><td>17.672</td><td>22.315</td></tr> <tr><td>6</td><td>-8.4</td><td>24.710</td><td>26.784</td></tr> <tr><td>7</td><td>-8.4</td><td>22.296</td><td>24.988</td></tr> <tr><td>8</td><td>-8.4</td><td>15.295</td><td>17.955</td></tr> <tr><td>9</td><td>-8.4</td><td>27.110</td><td>29.871</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-9.2	0.000	0.000	2	-9.1	2.644	9.430	3	-9.0	15.398	17.005	4	-8.9	24.686	27.320	5	-8.5	17.672	22.315	6	-8.4	24.710	26.784	7	-8.4	22.296	24.988	8	-8.4	15.295	17.955	9	-8.4	27.110	29.871
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4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- Present in (ASO, AWSO)	Compound CID: 119838	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-5.5</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-5.3</td><td>17.864</td><td>19.012</td></tr> <tr><td>3</td><td>-5.0</td><td>18.386</td><td>19.576</td></tr> <tr><td>4</td><td>-4.9</td><td>17.778</td><td>18.814</td></tr> <tr><td>5</td><td>-4.8</td><td>12.791</td><td>13.765</td></tr> <tr><td>6</td><td>-4.7</td><td>13.006</td><td>13.807</td></tr> <tr><td>7</td><td>-4.7</td><td>11.981</td><td>12.892</td></tr> <tr><td>8</td><td>-4.7</td><td>13.504</td><td>14.690</td></tr> <tr><td>9</td><td>-4.7</td><td>14.464</td><td>15.373</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-5.5	0.000	0.000	2	-5.3	17.864	19.012	3	-5.0	18.386	19.576	4	-4.9	17.778	18.814	5	-4.8	12.791	13.765	6	-4.7	13.006	13.807	7	-4.7	11.981	12.892	8	-4.7	13.504	14.690	9	-4.7	14.464	15.373	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-5.5</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-5.5</td><td>1.117</td><td>2.321</td></tr> <tr><td>3</td><td>-5.4</td><td>0.841</td><td>2.691</td></tr> <tr><td>4</td><td>-5.3</td><td>27.393</td><td>28.279</td></tr> <tr><td>5</td><td>-5.3</td><td>1.358</td><td>3.186</td></tr> <tr><td>6</td><td>-5.2</td><td>27.459</td><td>28.468</td></tr> <tr><td>7</td><td>-5.1</td><td>28.899</td><td>29.664</td></tr> <tr><td>8</td><td>-4.9</td><td>28.793</td><td>29.736</td></tr> <tr><td>9</td><td>-4.9</td><td>20.258</td><td>20.627</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-5.5	0.000	0.000	2	-5.5	1.117	2.321	3	-5.4	0.841	2.691	4	-5.3	27.393	28.279	5	-5.3	1.358	3.186	6	-5.2	27.459	28.468	7	-5.1	28.899	29.664	8	-4.9	28.793	29.736	9	-4.9	20.258	20.627
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5-Hydroxymethylfurfural Present in (AWSO)	Compound CID: 237332	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-5.2</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-5.2</td><td>0.186</td><td>3.024</td></tr> <tr><td>3</td><td>-4.8</td><td>13.344</td><td>14.578</td></tr> <tr><td>4</td><td>-4.7</td><td>13.219</td><td>14.517</td></tr> <tr><td>5</td><td>-4.6</td><td>13.612</td><td>14.414</td></tr> <tr><td>6</td><td>-4.5</td><td>13.256</td><td>14.582</td></tr> <tr><td>7</td><td>-4.4</td><td>13.776</td><td>14.425</td></tr> <tr><td>8</td><td>-4.4</td><td>13.828</td><td>14.535</td></tr> <tr><td>9</td><td>-4.2</td><td>14.073</td><td>15.062</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-5.2	0.000	0.000	2	-5.2	0.186	3.024	3	-4.8	13.344	14.578	4	-4.7	13.219	14.517	5	-4.6	13.612	14.414	6	-4.5	13.256	14.582	7	-4.4	13.776	14.425	8	-4.4	13.828	14.535	9	-4.2	14.073	15.062	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-5.8</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-5.5</td><td>26.510</td><td>27.617</td></tr> <tr><td>3</td><td>-5.5</td><td>26.719</td><td>27.753</td></tr> <tr><td>4</td><td>-5.5</td><td>0.986</td><td>3.202</td></tr> <tr><td>5</td><td>-5.2</td><td>27.532</td><td>28.651</td></tr> <tr><td>6</td><td>-5.2</td><td>15.303</td><td>15.648</td></tr> <tr><td>7</td><td>-5.2</td><td>27.167</td><td>28.172</td></tr> <tr><td>8</td><td>-4.6</td><td>15.355</td><td>16.075</td></tr> <tr><td>9</td><td>-4.6</td><td>1.932</td><td>2.470</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-5.8	0.000	0.000	2	-5.5	26.510	27.617	3	-5.5	26.719	27.753	4	-5.5	0.986	3.202	5	-5.2	27.532	28.651	6	-5.2	15.303	15.648	7	-5.2	27.167	28.172	8	-4.6	15.355	16.075	9	-4.6	1.932	2.470
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Oleic Acid Present in AWSO, AVSO	Compound CID: 445639	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-6.9</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.6</td><td>4.399</td><td>8.852</td></tr> <tr><td>3</td><td>-6.4</td><td>15.927</td><td>16.746</td></tr> <tr><td>4</td><td>-6.3</td><td>28.681</td><td>29.084</td></tr> <tr><td>5</td><td>-6.2</td><td>20.984</td><td>22.463</td></tr> <tr><td>6</td><td>-6.2</td><td>28.048</td><td>29.481</td></tr> <tr><td>7</td><td>-6.2</td><td>16.235</td><td>17.572</td></tr> <tr><td>8</td><td>-5.9</td><td>6.599</td><td>10.502</td></tr> <tr><td>9</td><td>-5.9</td><td>15.853</td><td>19.377</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-6.9	0.000	0.000	2	-6.6	4.399	8.852	3	-6.4	15.927	16.746	4	-6.3	28.681	29.084	5	-6.2	20.984	22.463	6	-6.2	28.048	29.481	7	-6.2	16.235	17.572	8	-5.9	6.599	10.502	9	-5.9	15.853	19.377	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-7.5</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.8</td><td>4.558</td><td>9.365</td></tr> <tr><td>3</td><td>-6.5</td><td>18.853</td><td>22.382</td></tr> <tr><td>4</td><td>-6.3</td><td>14.528</td><td>15.967</td></tr> <tr><td>5</td><td>-6.2</td><td>24.855</td><td>25.820</td></tr> <tr><td>6</td><td>-6.1</td><td>36.732</td><td>38.955</td></tr> <tr><td>7</td><td>-5.9</td><td>26.175</td><td>27.146</td></tr> <tr><td>8</td><td>-5.9</td><td>15.952</td><td>19.751</td></tr> <tr><td>9</td><td>-5.8</td><td>5.048</td><td>9.615</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-7.5	0.000	0.000	2	-6.8	4.558	9.365	3	-6.5	18.853	22.382	4	-6.3	14.528	15.967	5	-6.2	24.855	25.820	6	-6.1	36.732	38.955	7	-5.9	26.175	27.146	8	-5.9	15.952	19.751	9	-5.8	5.048	9.615
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Compounds separated by GC-MS	Chemical (PubChem CID:)	AutoDock analysis results with 2rh1	AutoDock analysis results with 3D0G																																																																																
.alpha.-D-Glucopyranoside, O-.alpha.-D-glucopyranosyl-(1.fwdarw.3)-.beta.-D-fructofuranosyl Present in AWSO	Compound CID: 220003	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-9.0</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-8.7</td><td>0.845</td><td>1.773</td></tr> <tr><td>3</td><td>-8.4</td><td>2.565</td><td>5.571</td></tr> <tr><td>4</td><td>-8.3</td><td>1.888</td><td>2.978</td></tr> <tr><td>5</td><td>-8.1</td><td>2.292</td><td>5.704</td></tr> <tr><td>6</td><td>-8.1</td><td>2.098</td><td>2.476</td></tr> <tr><td>7</td><td>-8.1</td><td>2.411</td><td>4.062</td></tr> <tr><td>8</td><td>-8.0</td><td>2.623</td><td>5.659</td></tr> <tr><td>9</td><td>-8.0</td><td>1.950</td><td>5.032</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	best mode rmsd u.b.	1	-9.0	0.000	0.000	2	-8.7	0.845	1.773	3	-8.4	2.565	5.571	4	-8.3	1.888	2.978	5	-8.1	2.292	5.704	6	-8.1	2.098	2.476	7	-8.1	2.411	4.062	8	-8.0	2.623	5.659	9	-8.0	1.950	5.032	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-9.2</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-8.9</td><td>0.926</td><td>2.318</td></tr> <tr><td>3</td><td>-8.7</td><td>1.659</td><td>6.107</td></tr> <tr><td>4</td><td>-8.6</td><td>1.628</td><td>3.081</td></tr> <tr><td>5</td><td>-8.5</td><td>1.834</td><td>3.344</td></tr> <tr><td>6</td><td>-8.3</td><td>1.870</td><td>2.887</td></tr> <tr><td>7</td><td>-8.1</td><td>28.229</td><td>32.382</td></tr> <tr><td>8</td><td>-8.0</td><td>21.065</td><td>22.693</td></tr> <tr><td>9</td><td>-7.9</td><td>24.724</td><td>28.286</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	best mode rmsd u.b.	1	-9.2	0.000	0.000	2	-8.9	0.926	2.318	3	-8.7	1.659	6.107	4	-8.6	1.628	3.081	5	-8.5	1.834	3.344	6	-8.3	1.870	2.887	7	-8.1	28.229	32.382	8	-8.0	21.065	22.693	9	-7.9	24.724	28.286
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8	-8.0	2.623	5.659																																																																																
9	-8.0	1.950	5.032																																																																																
mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	best mode rmsd u.b.																																																																																
1	-9.2	0.000	0.000																																																																																
2	-8.9	0.926	2.318																																																																																
3	-8.7	1.659	6.107																																																																																
4	-8.6	1.628	3.081																																																																																
5	-8.5	1.834	3.344																																																																																
6	-8.3	1.870	2.887																																																																																
7	-8.1	28.229	32.382																																																																																
8	-8.0	21.065	22.693																																																																																
9	-7.9	24.724	28.286																																																																																
Palmitic Acid Present in AWSO	Compound CID: 985	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-6.2</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.1</td><td>29.184</td><td>30.283</td></tr> <tr><td>3</td><td>-6.0</td><td>28.408</td><td>29.564</td></tr> <tr><td>4</td><td>-6.0</td><td>1.387</td><td>2.887</td></tr> <tr><td>5</td><td>-5.9</td><td>29.258</td><td>30.780</td></tr> <tr><td>6</td><td>-5.9</td><td>32.407</td><td>33.522</td></tr> <tr><td>7</td><td>-5.6</td><td>17.916</td><td>18.875</td></tr> <tr><td>8</td><td>-5.5</td><td>28.751</td><td>29.877</td></tr> <tr><td>9</td><td>-5.4</td><td>28.634</td><td>30.111</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	best mode rmsd u.b.	1	-6.2	0.000	0.000	2	-6.1	29.184	30.283	3	-6.0	28.408	29.564	4	-6.0	1.387	2.887	5	-5.9	29.258	30.780	6	-5.9	32.407	33.522	7	-5.6	17.916	18.875	8	-5.5	28.751	29.877	9	-5.4	28.634	30.111	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-6.8</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.7</td><td>4.216</td><td>8.437</td></tr> <tr><td>3</td><td>-6.5</td><td>3.238</td><td>5.240</td></tr> <tr><td>4</td><td>-5.8</td><td>19.657</td><td>23.031</td></tr> <tr><td>5</td><td>-5.6</td><td>24.575</td><td>25.488</td></tr> <tr><td>6</td><td>-5.5</td><td>14.299</td><td>16.135</td></tr> <tr><td>7</td><td>-5.4</td><td>25.853</td><td>26.594</td></tr> <tr><td>8</td><td>-5.3</td><td>14.432</td><td>18.616</td></tr> <tr><td>9</td><td>-5.2</td><td>3.647</td><td>6.484</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	best mode rmsd u.b.	1	-6.8	0.000	0.000	2	-6.7	4.216	8.437	3	-6.5	3.238	5.240	4	-5.8	19.657	23.031	5	-5.6	24.575	25.488	6	-5.5	14.299	16.135	7	-5.4	25.853	26.594	8	-5.3	14.432	18.616	9	-5.2	3.647	6.484
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9	-5.2	3.647	6.484																																																																																
Levoglucosenone Present in AWSO	Compound CID: 699486	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-4.8</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-4.7</td><td>13.323</td><td>14.380</td></tr> <tr><td>3</td><td>-4.7</td><td>14.300</td><td>14.794</td></tr> <tr><td>4</td><td>-4.6</td><td>13.154</td><td>14.340</td></tr> <tr><td>5</td><td>-4.6</td><td>14.555</td><td>15.265</td></tr> <tr><td>6</td><td>-4.5</td><td>13.651</td><td>14.602</td></tr> <tr><td>7</td><td>-4.5</td><td>17.497</td><td>18.356</td></tr> <tr><td>8</td><td>-4.5</td><td>12.905</td><td>13.874</td></tr> <tr><td>9</td><td>-4.4</td><td>13.480</td><td>14.464</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	best mode rmsd u.b.	1	-4.8	0.000	0.000	2	-4.7	13.323	14.380	3	-4.7	14.300	14.794	4	-4.6	13.154	14.340	5	-4.6	14.555	15.265	6	-4.5	13.651	14.602	7	-4.5	17.497	18.356	8	-4.5	12.905	13.874	9	-4.4	13.480	14.464	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-5.5</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-5.3</td><td>1.017</td><td>3.019</td></tr> <tr><td>3</td><td>-4.9</td><td>16.326</td><td>17.014</td></tr> <tr><td>4</td><td>-4.8</td><td>2.042</td><td>3.201</td></tr> <tr><td>5</td><td>-4.8</td><td>16.520</td><td>17.277</td></tr> <tr><td>6</td><td>-4.8</td><td>1.609</td><td>3.148</td></tr> <tr><td>7</td><td>-4.6</td><td>19.577</td><td>20.518</td></tr> <tr><td>8</td><td>-4.6</td><td>17.032</td><td>17.638</td></tr> <tr><td>9</td><td>-4.6</td><td>17.881</td><td>18.350</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	best mode rmsd u.b.	1	-5.5	0.000	0.000	2	-5.3	1.017	3.019	3	-4.9	16.326	17.014	4	-4.8	2.042	3.201	5	-4.8	16.520	17.277	6	-4.8	1.609	3.148	7	-4.6	19.577	20.518	8	-4.6	17.032	17.638	9	-4.6	17.881	18.350
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Cyclopropanecarboxylic acid, 3-formyl-2,2-dimethyl-, ethyl ester Present in AWSO	Compound CID: 566079	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-5.5</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-5.4</td><td>17.177</td><td>18.084</td></tr> <tr><td>3</td><td>-5.4</td><td>10.237</td><td>10.930</td></tr> <tr><td>4</td><td>-5.3</td><td>15.707</td><td>16.560</td></tr> <tr><td>5</td><td>-5.3</td><td>16.494</td><td>17.431</td></tr> <tr><td>6</td><td>-5.3</td><td>1.228</td><td>3.615</td></tr> <tr><td>7</td><td>-5.3</td><td>13.153</td><td>13.611</td></tr> <tr><td>8</td><td>-5.3</td><td>15.377</td><td>16.280</td></tr> <tr><td>9</td><td>-5.2</td><td>12.978</td><td>13.888</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	best mode rmsd u.b.	1	-5.5	0.000	0.000	2	-5.4	17.177	18.084	3	-5.4	10.237	10.930	4	-5.3	15.707	16.560	5	-5.3	16.494	17.431	6	-5.3	1.228	3.615	7	-5.3	13.153	13.611	8	-5.3	15.377	16.280	9	-5.2	12.978	13.888	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-5.9</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-5.8</td><td>1.255</td><td>1.847</td></tr> <tr><td>3</td><td>-5.8</td><td>1.818</td><td>2.424</td></tr> <tr><td>4</td><td>-5.5</td><td>26.325</td><td>27.585</td></tr> <tr><td>5</td><td>-5.5</td><td>37.958</td><td>39.170</td></tr> <tr><td>6</td><td>-5.4</td><td>35.685</td><td>37.746</td></tr> <tr><td>7</td><td>-5.4</td><td>1.347</td><td>3.136</td></tr> <tr><td>8</td><td>-5.4</td><td>25.450</td><td>26.330</td></tr> <tr><td>9</td><td>-5.3</td><td>35.977</td><td>37.769</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	best mode rmsd u.b.	1	-5.9	0.000	0.000	2	-5.8	1.255	1.847	3	-5.8	1.818	2.424	4	-5.5	26.325	27.585	5	-5.5	37.958	39.170	6	-5.4	35.685	37.746	7	-5.4	1.347	3.136	8	-5.4	25.450	26.330	9	-5.3	35.977	37.769
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1H-Inden-1-ol, 2,3-dihydro- Present in AWSO	Compound CID: 22819	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-6.4</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.3</td><td>12.710</td><td>13.701</td></tr> <tr><td>3</td><td>-6.2</td><td>0.827</td><td>1.591</td></tr> <tr><td>4</td><td>-6.1</td><td>1.304</td><td>1.918</td></tr> <tr><td>5</td><td>-6.1</td><td>1.437</td><td>2.851</td></tr> <tr><td>6</td><td>-6.0</td><td>1.276</td><td>2.311</td></tr> <tr><td>7</td><td>-5.8</td><td>15.442</td><td>16.251</td></tr> <tr><td>8</td><td>-5.4</td><td>15.889</td><td>16.886</td></tr> <tr><td>9</td><td>-5.4</td><td>16.307</td><td>17.305</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	best mode rmsd u.b.	1	-6.4	0.000	0.000	2	-6.3	12.710	13.701	3	-6.2	0.827	1.591	4	-6.1	1.304	1.918	5	-6.1	1.437	2.851	6	-6.0	1.276	2.311	7	-5.8	15.442	16.251	8	-5.4	15.889	16.886	9	-5.4	16.307	17.305	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-8.1</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-7.9</td><td>1.508</td><td>2.882</td></tr> <tr><td>3</td><td>-7.0</td><td>18.232</td><td>19.432</td></tr> <tr><td>4</td><td>-6.8</td><td>1.593</td><td>2.663</td></tr> <tr><td>5</td><td>-6.6</td><td>27.095</td><td>27.934</td></tr> <tr><td>6</td><td>-6.4</td><td>18.143</td><td>19.531</td></tr> <tr><td>7</td><td>-6.0</td><td>27.051</td><td>27.955</td></tr> <tr><td>8</td><td>-5.9</td><td>15.508</td><td>16.036</td></tr> <tr><td>9</td><td>-5.8</td><td>27.575</td><td>28.466</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	best mode rmsd u.b.	1	-8.1	0.000	0.000	2	-7.9	1.508	2.882	3	-7.0	18.232	19.432	4	-6.8	1.593	2.663	5	-6.6	27.095	27.934	6	-6.4	18.143	19.531	7	-6.0	27.051	27.955	8	-5.9	15.508	16.036	9	-5.8	27.575	28.466
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Phenol, 2,6-bis(1,1-dimethylethyl)- Present in AWSO	Compound CID: 31405	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-7.5</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-7.5</td><td>17.582</td><td>19.509</td></tr> <tr><td>3</td><td>-7.4</td><td>0.868</td><td>3.953</td></tr> <tr><td>4</td><td>-7.2</td><td>2.719</td><td>4.137</td></tr> <tr><td>5</td><td>-7.2</td><td>14.465</td><td>15.405</td></tr> <tr><td>6</td><td>-7.1</td><td>18.104</td><td>19.251</td></tr> <tr><td>7</td><td>-7.1</td><td>2.592</td><td>3.184</td></tr> <tr><td>8</td><td>-6.9</td><td>2.775</td><td>4.408</td></tr> <tr><td>9</td><td>-6.9</td><td>14.391</td><td>16.477</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	best mode rmsd u.b.	1	-7.5	0.000	0.000	2	-7.5	17.582	19.509	3	-7.4	0.868	3.953	4	-7.2	2.719	4.137	5	-7.2	14.465	15.405	6	-7.1	18.104	19.251	7	-7.1	2.592	3.184	8	-6.9	2.775	4.408	9	-6.9	14.391	16.477	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>best mode rmsd u.b.</th></tr> <tr><td>1</td><td>-9.2</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-9.0</td><td>0.796</td><td>3.944</td></tr> <tr><td>3</td><td>-7.6</td><td>1.502</td><td>2.072</td></tr> <tr><td>4</td><td>-7.3</td><td>1.891</td><td>3.087</td></tr> <tr><td>5</td><td>-7.3</td><td>1.264</td><td>4.535</td></tr> <tr><td>6</td><td>-7.0</td><td>38.053</td><td>39.177</td></tr> <tr><td>7</td><td>-7.0</td><td>1.945</td><td>3.277</td></tr> <tr><td>8</td><td>-6.9</td><td>11.983</td><td>14.086</td></tr> <tr><td>9</td><td>-6.9</td><td>11.905</td><td>14.214</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	best mode rmsd u.b.	1	-9.2	0.000	0.000	2	-9.0	0.796	3.944	3	-7.6	1.502	2.072	4	-7.3	1.891	3.087	5	-7.3	1.264	4.535	6	-7.0	38.053	39.177	7	-7.0	1.945	3.277	8	-6.9	11.983	14.086	9	-6.9	11.905	14.214
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Compounds separated by GC-MS	Chemical (PubChem CID:)	AutoDock analysis results with 2rh1	AutoDock analysis results with 3D0G																																																																																
Chloro(2-methyloxiran-2-yl)acetic acid, t-butyl ester Present in AWSO	Compound CID: 545402	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-6.1</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.1</td><td>1.942</td><td>2.421</td></tr> <tr><td>3</td><td>-6.0</td><td>2.048</td><td>2.789</td></tr> <tr><td>4</td><td>-5.9</td><td>1.453</td><td>3.407</td></tr> <tr><td>5</td><td>-5.9</td><td>20.214</td><td>20.814</td></tr> <tr><td>6</td><td>-5.9</td><td>1.929</td><td>3.496</td></tr> <tr><td>7</td><td>-5.9</td><td>2.073</td><td>3.229</td></tr> <tr><td>8</td><td>-5.8</td><td>1.896</td><td>2.286</td></tr> <tr><td>9</td><td>-5.7</td><td>19.777</td><td>21.084</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-6.1	0.000	0.000	2	-6.1	1.942	2.421	3	-6.0	2.048	2.789	4	-5.9	1.453	3.407	5	-5.9	20.214	20.814	6	-5.9	1.929	3.496	7	-5.9	2.073	3.229	8	-5.8	1.896	2.286	9	-5.7	19.777	21.084	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-6.6</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.4</td><td>17.353</td><td>18.028</td></tr> <tr><td>3</td><td>-6.1</td><td>27.462</td><td>28.697</td></tr> <tr><td>4</td><td>-6.1</td><td>27.706</td><td>28.726</td></tr> <tr><td>5</td><td>-6.1</td><td>1.337</td><td>3.409</td></tr> <tr><td>6</td><td>-5.8</td><td>26.519</td><td>27.548</td></tr> <tr><td>7</td><td>-5.6</td><td>2.127</td><td>3.245</td></tr> <tr><td>8</td><td>-5.6</td><td>17.193</td><td>17.875</td></tr> <tr><td>9</td><td>-5.4</td><td>17.528</td><td>18.591</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-6.6	0.000	0.000	2	-6.4	17.353	18.028	3	-6.1	27.462	28.697	4	-6.1	27.706	28.726	5	-6.1	1.337	3.409	6	-5.8	26.519	27.548	7	-5.6	2.127	3.245	8	-5.6	17.193	17.875	9	-5.4	17.528	18.591
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Cyclodecacyclododecene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18-octadecahydro- Present in AVSO	Compound CID: 5377998	<table> <tr> <th>ode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-10.2</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-10.2</td><td>0.523</td><td>4.721</td></tr> <tr><td>3</td><td>-9.9</td><td>17.642</td><td>19.657</td></tr> <tr><td>4</td><td>-9.8</td><td>3.490</td><td>4.954</td></tr> <tr><td>5</td><td>-9.8</td><td>20.800</td><td>22.429</td></tr> <tr><td>6</td><td>-9.7</td><td>2.296</td><td>3.959</td></tr> <tr><td>7</td><td>-9.6</td><td>0.993</td><td>5.158</td></tr> <tr><td>8</td><td>-9.6</td><td>1.652</td><td>5.058</td></tr> <tr><td>9</td><td>-9.3</td><td>3.728</td><td>4.464</td></tr> </table>	ode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-10.2	0.000	0.000	2	-10.2	0.523	4.721	3	-9.9	17.642	19.657	4	-9.8	3.490	4.954	5	-9.8	20.800	22.429	6	-9.7	2.296	3.959	7	-9.6	0.993	5.158	8	-9.6	1.652	5.058	9	-9.3	3.728	4.464	<table> <tr> <th>ode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-10.9</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-10.8</td><td>0.778</td><td>4.722</td></tr> <tr><td>3</td><td>-10.6</td><td>1.433</td><td>5.216</td></tr> <tr><td>4</td><td>-10.1</td><td>1.585</td><td>2.999</td></tr> <tr><td>5</td><td>-9.6</td><td>1.803</td><td>4.453</td></tr> <tr><td>6</td><td>-9.4</td><td>38.573</td><td>40.881</td></tr> <tr><td>7</td><td>-9.3</td><td>35.086</td><td>37.269</td></tr> <tr><td>8</td><td>-9.3</td><td>1.327</td><td>2.795</td></tr> <tr><td>9</td><td>-9.2</td><td>38.634</td><td>41.051</td></tr> </table>	ode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-10.9	0.000	0.000	2	-10.8	0.778	4.722	3	-10.6	1.433	5.216	4	-10.1	1.585	2.999	5	-9.6	1.803	4.453	6	-9.4	38.573	40.881	7	-9.3	35.086	37.269	8	-9.3	1.327	2.795	9	-9.2	38.634	41.051
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2H-Pyran, 2-(7-heptadecynyloxy)tetrahydro- Present in AVSO	Compound CID: 543312	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-6.6</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.6</td><td>3.582</td><td>10.924</td></tr> <tr><td>3</td><td>-6.3</td><td>16.531</td><td>20.334</td></tr> <tr><td>4</td><td>-6.1</td><td>16.684</td><td>19.519</td></tr> <tr><td>5</td><td>-6.0</td><td>2.977</td><td>10.224</td></tr> <tr><td>6</td><td>-6.0</td><td>27.886</td><td>30.156</td></tr> <tr><td>7</td><td>-5.8</td><td>3.824</td><td>5.162</td></tr> <tr><td>8</td><td>-5.8</td><td>16.867</td><td>18.807</td></tr> <tr><td>9</td><td>-5.8</td><td>16.728</td><td>19.851</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-6.6	0.000	0.000	2	-6.6	3.582	10.924	3	-6.3	16.531	20.334	4	-6.1	16.684	19.519	5	-6.0	2.977	10.224	6	-6.0	27.886	30.156	7	-5.8	3.824	5.162	8	-5.8	16.867	18.807	9	-5.8	16.728	19.851	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-6.2</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.0</td><td>40.198</td><td>43.433</td></tr> <tr><td>3</td><td>-5.9</td><td>0.985</td><td>2.935</td></tr> <tr><td>4</td><td>-5.9</td><td>41.743</td><td>44.146</td></tr> <tr><td>5</td><td>-5.8</td><td>37.624</td><td>40.095</td></tr> <tr><td>6</td><td>-5.5</td><td>27.873</td><td>32.299</td></tr> <tr><td>7</td><td>-5.4</td><td>1.421</td><td>1.568</td></tr> <tr><td>8</td><td>-5.2</td><td>31.991</td><td>33.836</td></tr> <tr><td>9</td><td>-5.2</td><td>26.014</td><td>31.189</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-6.2	0.000	0.000	2	-6.0	40.198	43.433	3	-5.9	0.985	2.935	4	-5.9	41.743	44.146	5	-5.8	37.624	40.095	6	-5.5	27.873	32.299	7	-5.4	1.421	1.568	8	-5.2	31.991	33.836	9	-5.2	26.014	31.189
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Androstan-17-one, 3-ethyl-3-hydroxy-, (5.alpha.)- Present in AVSO	Compound CID: 14681481	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-10.7</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-10.4</td><td>14.744</td><td>16.048</td></tr> <tr><td>3</td><td>-10.3</td><td>3.439</td><td>4.561</td></tr> <tr><td>4</td><td>-10.1</td><td>3.544</td><td>4.729</td></tr> <tr><td>5</td><td>-10.0</td><td>15.536</td><td>17.423</td></tr> <tr><td>6</td><td>-9.8</td><td>2.512</td><td>4.669</td></tr> <tr><td>7</td><td>-9.8</td><td>11.855</td><td>14.364</td></tr> <tr><td>8</td><td>-9.7</td><td>3.649</td><td>4.254</td></tr> <tr><td>9</td><td>-9.6</td><td>14.528</td><td>16.749</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-10.7	0.000	0.000	2	-10.4	14.744	16.048	3	-10.3	3.439	4.561	4	-10.1	3.544	4.729	5	-10.0	15.536	17.423	6	-9.8	2.512	4.669	7	-9.8	11.855	14.364	8	-9.7	3.649	4.254	9	-9.6	14.528	16.749	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-11.5</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-11.4</td><td>0.775</td><td>5.222</td></tr> <tr><td>3</td><td>-11.2</td><td>0.752</td><td>4.921</td></tr> <tr><td>4</td><td>-10.5</td><td>1.603</td><td>1.881</td></tr> <tr><td>5</td><td>-9.9</td><td>12.299</td><td>14.850</td></tr> <tr><td>6</td><td>-9.6</td><td>2.401</td><td>4.506</td></tr> <tr><td>7</td><td>-9.5</td><td>1.770</td><td>5.443</td></tr> <tr><td>8</td><td>-9.0</td><td>3.011</td><td>4.555</td></tr> <tr><td>9</td><td>-8.9</td><td>2.949</td><td>5.366</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-11.5	0.000	0.000	2	-11.4	0.775	5.222	3	-11.2	0.752	4.921	4	-10.5	1.603	1.881	5	-9.9	12.299	14.850	6	-9.6	2.401	4.506	7	-9.5	1.770	5.443	8	-9.0	3.011	4.555	9	-8.9	2.949	5.366
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mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.																																																																																
1	-11.5	0.000	0.000																																																																																
2	-11.4	0.775	5.222																																																																																
3	-11.2	0.752	4.921																																																																																
4	-10.5	1.603	1.881																																																																																
5	-9.9	12.299	14.850																																																																																
6	-9.6	2.401	4.506																																																																																
7	-9.5	1.770	5.443																																																																																
8	-9.0	3.011	4.555																																																																																
9	-8.9	2.949	5.366																																																																																
Z,E-2,13-Octadecadien-1-ol Present in AVSO	Compound CID: 5364462	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-6.7</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.3</td><td>16.407</td><td>18.939</td></tr> <tr><td>3</td><td>-6.3</td><td>15.604</td><td>18.162</td></tr> <tr><td>4</td><td>-6.3</td><td>15.525</td><td>18.036</td></tr> <tr><td>5</td><td>-6.2</td><td>6.453</td><td>7.028</td></tr> <tr><td>6</td><td>-6.2</td><td>16.176</td><td>18.786</td></tr> <tr><td>7</td><td>-6.1</td><td>15.982</td><td>18.486</td></tr> <tr><td>8</td><td>-6.1</td><td>17.263</td><td>19.792</td></tr> <tr><td>9</td><td>-6.0</td><td>2.498</td><td>7.773</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-6.7	0.000	0.000	2	-6.3	16.407	18.939	3	-6.3	15.604	18.162	4	-6.3	15.525	18.036	5	-6.2	6.453	7.028	6	-6.2	16.176	18.786	7	-6.1	15.982	18.486	8	-6.1	17.263	19.792	9	-6.0	2.498	7.773	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-6.9</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.7</td><td>40.178</td><td>42.364</td></tr> <tr><td>3</td><td>-6.5</td><td>2.359</td><td>2.557</td></tr> <tr><td>4</td><td>-6.3</td><td>21.526</td><td>22.832</td></tr> <tr><td>5</td><td>-6.3</td><td>20.990</td><td>22.429</td></tr> <tr><td>6</td><td>-6.2</td><td>19.788</td><td>22.816</td></tr> <tr><td>7</td><td>-6.1</td><td>25.086</td><td>29.196</td></tr> <tr><td>8</td><td>-6.1</td><td>1.800</td><td>2.120</td></tr> <tr><td>9</td><td>-6.1</td><td>31.805</td><td>33.274</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-6.9	0.000	0.000	2	-6.7	40.178	42.364	3	-6.5	2.359	2.557	4	-6.3	21.526	22.832	5	-6.3	20.990	22.429	6	-6.2	19.788	22.816	7	-6.1	25.086	29.196	8	-6.1	1.800	2.120	9	-6.1	31.805	33.274
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Chrysene, octadecahydro Present in AVSO	Compound CID: 98460	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-9.6</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-9.6</td><td>0.089</td><td>4.507</td></tr> <tr><td>3</td><td>-9.3</td><td>9.946</td><td>10.519</td></tr> <tr><td>4</td><td>-9.3</td><td>9.933</td><td>10.472</td></tr> <tr><td>5</td><td>-9.3</td><td>20.482</td><td>21.705</td></tr> <tr><td>6</td><td>-9.2</td><td>20.473</td><td>21.756</td></tr> <tr><td>7</td><td>-9.1</td><td>17.752</td><td>19.621</td></tr> <tr><td>8</td><td>-9.1</td><td>17.950</td><td>19.561</td></tr> <tr><td>9</td><td>-9.0</td><td>9.827</td><td>10.653</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-9.6	0.000	0.000	2	-9.6	0.089	4.507	3	-9.3	9.946	10.519	4	-9.3	9.933	10.472	5	-9.3	20.482	21.705	6	-9.2	20.473	21.756	7	-9.1	17.752	19.621	8	-9.1	17.950	19.561	9	-9.0	9.827	10.653	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-11.5</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-11.2</td><td>0.085</td><td>4.507</td></tr> <tr><td>3</td><td>-11.1</td><td>0.596</td><td>1.901</td></tr> <tr><td>4</td><td>-10.5</td><td>0.533</td><td>4.115</td></tr> <tr><td>5</td><td>-9.0</td><td>1.729</td><td>3.305</td></tr> <tr><td>6</td><td>-8.9</td><td>1.493</td><td>4.295</td></tr> <tr><td>7</td><td>-8.9</td><td>1.735</td><td>3.760</td></tr> <tr><td>8</td><td>-8.5</td><td>41.958</td><td>43.502</td></tr> <tr><td>9</td><td>-8.3</td><td>12.082</td><td>14.471</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-11.5	0.000	0.000	2	-11.2	0.085	4.507	3	-11.1	0.596	1.901	4	-10.5	0.533	4.115	5	-9.0	1.729	3.305	6	-8.9	1.493	4.295	7	-8.9	1.735	3.760	8	-8.5	41.958	43.502	9	-8.3	12.082	14.471
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Compounds separated by GC-MS	Chemical (PubChem CID:)	AutoDock analysis results with 2rh1	AutoDock analysis results with 3D0G																																																																																
Bicyclo[10.6.0]octadeca-1(12),15-diene Present in AVSO	Compound CID: 5362802	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-9.2</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-9.2</td><td>0.326</td><td>2.147</td></tr> <tr><td>3</td><td>-9.2</td><td>17.079</td><td>18.646</td></tr> <tr><td>4</td><td>-9.0</td><td>15.091</td><td>16.643</td></tr> <tr><td>5</td><td>-9.0</td><td>14.309</td><td>16.332</td></tr> <tr><td>6</td><td>-8.9</td><td>16.041</td><td>18.057</td></tr> <tr><td>7</td><td>-8.9</td><td>9.646</td><td>10.280</td></tr> <tr><td>8</td><td>-8.8</td><td>16.065</td><td>18.014</td></tr> <tr><td>9</td><td>-8.8</td><td>16.123</td><td>17.626</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-9.2	0.000	0.000	2	-9.2	0.326	2.147	3	-9.2	17.079	18.646	4	-9.0	15.091	16.643	5	-9.0	14.309	16.332	6	-8.9	16.041	18.057	7	-8.9	9.646	10.280	8	-8.8	16.065	18.014	9	-8.8	16.123	17.626	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-10.6</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-10.0</td><td>0.977</td><td>2.379</td></tr> <tr><td>3</td><td>-9.4</td><td>0.519</td><td>4.939</td></tr> <tr><td>4</td><td>-9.3</td><td>0.576</td><td>4.445</td></tr> <tr><td>5</td><td>-9.0</td><td>1.971</td><td>3.321</td></tr> <tr><td>6</td><td>-9.0</td><td>1.879</td><td>3.482</td></tr> <tr><td>7</td><td>-8.7</td><td>39.473</td><td>41.161</td></tr> <tr><td>8</td><td>-8.2</td><td>35.620</td><td>37.725</td></tr> <tr><td>9</td><td>-8.2</td><td>39.986</td><td>41.831</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-10.6	0.000	0.000	2	-10.0	0.977	2.379	3	-9.4	0.519	4.939	4	-9.3	0.576	4.445	5	-9.0	1.971	3.321	6	-9.0	1.879	3.482	7	-8.7	39.473	41.161	8	-8.2	35.620	37.725	9	-8.2	39.986	41.831
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3-Chloropropionic acid, heptadecyl ester Present in AVSO	Compound CID: 545757	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-7.4</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-7.1</td><td>16.925</td><td>18.312</td></tr> <tr><td>3</td><td>-7.0</td><td>1.143</td><td>2.260</td></tr> <tr><td>4</td><td>-7.0</td><td>5.726</td><td>10.439</td></tr> <tr><td>5</td><td>-7.0</td><td>16.849</td><td>18.513</td></tr> <tr><td>6</td><td>-6.9</td><td>3.345</td><td>4.188</td></tr> <tr><td>7</td><td>-6.9</td><td>5.108</td><td>10.473</td></tr> <tr><td>8</td><td>-6.8</td><td>6.496</td><td>10.670</td></tr> <tr><td>9</td><td>-6.8</td><td>17.132</td><td>19.571</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-7.4	0.000	0.000	2	-7.1	16.925	18.312	3	-7.0	1.143	2.260	4	-7.0	5.726	10.439	5	-7.0	16.849	18.513	6	-6.9	3.345	4.188	7	-6.9	5.108	10.473	8	-6.8	6.496	10.670	9	-6.8	17.132	19.571	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-6.8</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.8</td><td>5.166</td><td>10.618</td></tr> <tr><td>3</td><td>-6.2</td><td>16.158</td><td>19.942</td></tr> <tr><td>4</td><td>-6.2</td><td>23.731</td><td>24.374</td></tr> <tr><td>5</td><td>-6.1</td><td>18.270</td><td>22.113</td></tr> <tr><td>6</td><td>-6.1</td><td>2.139</td><td>2.194</td></tr> <tr><td>7</td><td>-6.1</td><td>15.811</td><td>18.620</td></tr> <tr><td>8</td><td>-6.0</td><td>24.946</td><td>25.513</td></tr> <tr><td>9</td><td>-5.9</td><td>26.365</td><td>26.831</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-6.8	0.000	0.000	2	-6.8	5.166	10.618	3	-6.2	16.158	19.942	4	-6.2	23.731	24.374	5	-6.1	18.270	22.113	6	-6.1	2.139	2.194	7	-6.1	15.811	18.620	8	-6.0	24.946	25.513	9	-5.9	26.365	26.831
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1-Heptatriacotanol Present in AVSO	Compound CID: 537071	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-5.3</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-5.3</td><td>2.237</td><td>6.162</td></tr> <tr><td>3</td><td>-5.2</td><td>16.965</td><td>20.320</td></tr> <tr><td>4</td><td>-4.8</td><td>2.573</td><td>4.970</td></tr> <tr><td>5</td><td>-4.8</td><td>2.676</td><td>7.123</td></tr> <tr><td>6</td><td>-4.7</td><td>1.823</td><td>6.032</td></tr> <tr><td>7</td><td>-4.6</td><td>2.557</td><td>4.467</td></tr> <tr><td>8</td><td>-4.6</td><td>1.584</td><td>3.408</td></tr> <tr><td>9</td><td>-4.5</td><td>17.434</td><td>20.547</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-5.3	0.000	0.000	2	-5.3	2.237	6.162	3	-5.2	16.965	20.320	4	-4.8	2.573	4.970	5	-4.8	2.676	7.123	6	-4.7	1.823	6.032	7	-4.6	2.557	4.467	8	-4.6	1.584	3.408	9	-4.5	17.434	20.547	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-4.6</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-4.6</td><td>25.283</td><td>27.890</td></tr> <tr><td>3</td><td>-4.4</td><td>22.064</td><td>24.643</td></tr> <tr><td>4</td><td>-4.3</td><td>10.130</td><td>11.854</td></tr> <tr><td>5</td><td>-4.2</td><td>22.305</td><td>25.024</td></tr> <tr><td>6</td><td>-4.1</td><td>10.736</td><td>13.188</td></tr> <tr><td>7</td><td>-4.1</td><td>14.038</td><td>16.273</td></tr> <tr><td>8</td><td>-3.9</td><td>14.903</td><td>18.729</td></tr> <tr><td>9</td><td>-3.9</td><td>23.521</td><td>26.162</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-4.6	0.000	0.000	2	-4.6	25.283	27.890	3	-4.4	22.064	24.643	4	-4.3	10.130	11.854	5	-4.2	22.305	25.024	6	-4.1	10.736	13.188	7	-4.1	14.038	16.273	8	-3.9	14.903	18.729	9	-3.9	23.521	26.162
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13-Docosenamide, (Z)- Present in AVSO	Compound CID: 5365371	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-8.8</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-8.3</td><td>17.652</td><td>21.097</td></tr> <tr><td>3</td><td>-8.2</td><td>5.337</td><td>10.259</td></tr> <tr><td>4</td><td>-8.0</td><td>3.610</td><td>4.839</td></tr> <tr><td>5</td><td>-8.0</td><td>21.076</td><td>22.207</td></tr> <tr><td>6</td><td>-8.0</td><td>5.357</td><td>10.728</td></tr> <tr><td>7</td><td>-7.8</td><td>5.023</td><td>10.766</td></tr> <tr><td>8</td><td>-7.7</td><td>18.053</td><td>21.502</td></tr> <tr><td>9</td><td>-7.6</td><td>2.394</td><td>3.734</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-8.8	0.000	0.000	2	-8.3	17.652	21.097	3	-8.2	5.337	10.259	4	-8.0	3.610	4.839	5	-8.0	21.076	22.207	6	-8.0	5.357	10.728	7	-7.8	5.023	10.766	8	-7.7	18.053	21.502	9	-7.6	2.394	3.734	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-8.6</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-8.0</td><td>17.430</td><td>21.995</td></tr> <tr><td>3</td><td>-7.7</td><td>4.903</td><td>10.627</td></tr> <tr><td>4</td><td>-7.3</td><td>26.018</td><td>26.951</td></tr> <tr><td>5</td><td>-7.0</td><td>26.747</td><td>29.032</td></tr> <tr><td>6</td><td>-6.9</td><td>25.955</td><td>26.804</td></tr> <tr><td>7</td><td>-6.8</td><td>24.008</td><td>30.146</td></tr> <tr><td>8</td><td>-6.8</td><td>17.404</td><td>21.901</td></tr> <tr><td>9</td><td>-6.8</td><td>7.016</td><td>10.298</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-8.6	0.000	0.000	2	-8.0	17.430	21.995	3	-7.7	4.903	10.627	4	-7.3	26.018	26.951	5	-7.0	26.747	29.032	6	-6.9	25.955	26.804	7	-6.8	24.008	30.146	8	-6.8	17.404	21.901	9	-6.8	7.016	10.298
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Caryophyllene oxide Present in AVSO	Compound CID: 1742210	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-8.6</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-8.4</td><td>20.442</td><td>21.179</td></tr> <tr><td>3</td><td>-8.3</td><td>0.944</td><td>2.541</td></tr> <tr><td>4</td><td>-8.3</td><td>17.395</td><td>18.881</td></tr> <tr><td>5</td><td>-8.2</td><td>10.253</td><td>10.962</td></tr> <tr><td>6</td><td>-8.2</td><td>9.255</td><td>9.995</td></tr> <tr><td>7</td><td>-8.2</td><td>1.353</td><td>3.270</td></tr> <tr><td>8</td><td>-8.1</td><td>18.096</td><td>19.598</td></tr> <tr><td>9</td><td>-8.1</td><td>20.033</td><td>20.862</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-8.6	0.000	0.000	2	-8.4	20.442	21.179	3	-8.3	0.944	2.541	4	-8.3	17.395	18.881	5	-8.2	10.253	10.962	6	-8.2	9.255	9.995	7	-8.2	1.353	3.270	8	-8.1	18.096	19.598	9	-8.1	20.033	20.862	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-10.4</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-10.3</td><td>0.996</td><td>2.512</td></tr> <tr><td>3</td><td>-9.3</td><td>1.359</td><td>3.435</td></tr> <tr><td>4</td><td>-9.2</td><td>1.484</td><td>3.158</td></tr> <tr><td>5</td><td>-9.1</td><td>0.687</td><td>2.563</td></tr> <tr><td>6</td><td>-8.1</td><td>1.459</td><td>2.891</td></tr> <tr><td>7</td><td>-7.7</td><td>15.347</td><td>16.457</td></tr> <tr><td>8</td><td>-7.5</td><td>14.954</td><td>15.710</td></tr> <tr><td>9</td><td>-7.4</td><td>15.408</td><td>16.343</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-10.4	0.000	0.000	2	-10.3	0.996	2.512	3	-9.3	1.359	3.435	4	-9.2	1.484	3.158	5	-9.1	0.687	2.563	6	-8.1	1.459	2.891	7	-7.7	15.347	16.457	8	-7.5	14.954	15.710	9	-7.4	15.408	16.343
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Heptacosane Present in AVSO	Compound CID: 11636	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-5.9</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-5.8</td><td>16.100</td><td>19.313</td></tr> <tr><td>3</td><td>-5.8</td><td>17.124</td><td>19.529</td></tr> <tr><td>4</td><td>-5.8</td><td>16.267</td><td>18.256</td></tr> <tr><td>5</td><td>-5.7</td><td>16.093</td><td>18.951</td></tr> <tr><td>6</td><td>-5.7</td><td>2.532</td><td>6.661</td></tr> <tr><td>7</td><td>-5.7</td><td>17.538</td><td>20.161</td></tr> <tr><td>8</td><td>-5.6</td><td>1.954</td><td>6.578</td></tr> <tr><td>9</td><td>-5.6</td><td>3.027</td><td>9.757</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-5.9	0.000	0.000	2	-5.8	16.100	19.313	3	-5.8	17.124	19.529	4	-5.8	16.267	18.256	5	-5.7	16.093	18.951	6	-5.7	2.532	6.661	7	-5.7	17.538	20.161	8	-5.6	1.954	6.578	9	-5.6	3.027	9.757	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-5.0</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-4.7</td><td>1.308</td><td>2.645</td></tr> <tr><td>3</td><td>-4.5</td><td>1.628</td><td>4.947</td></tr> <tr><td>4</td><td>-4.4</td><td>1.512</td><td>3.422</td></tr> <tr><td>5</td><td>-4.4</td><td>18.631</td><td>21.985</td></tr> <tr><td>6</td><td>-4.3</td><td>22.432</td><td>25.952</td></tr> <tr><td>7</td><td>-4.3</td><td>18.817</td><td>21.866</td></tr> <tr><td>8</td><td>-4.1</td><td>33.147</td><td>36.192</td></tr> <tr><td>9</td><td>-4.1</td><td>23.808</td><td>26.831</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-5.0	0.000	0.000	2	-4.7	1.308	2.645	3	-4.5	1.628	4.947	4	-4.4	1.512	3.422	5	-4.4	18.631	21.985	6	-4.3	22.432	25.952	7	-4.3	18.817	21.866	8	-4.1	33.147	36.192	9	-4.1	23.808	26.831
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Compounds separated by GC-MS	Chemical (PubChem CID:)	AutoDock analysis results with 2rh1	AutoDock analysis results with 3D0G																																																																																
.gamma.-Tocophero Present in AVSO	Compound CID: 91738518	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-10.0</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-9.9</td><td>2.235</td><td>3.863</td></tr> <tr><td>3</td><td>-9.8</td><td>27.078</td><td>28.146</td></tr> <tr><td>4</td><td>-9.6</td><td>1.500</td><td>2.645</td></tr> <tr><td>5</td><td>-9.4</td><td>20.786</td><td>23.827</td></tr> <tr><td>6</td><td>-9.4</td><td>20.388</td><td>24.313</td></tr> <tr><td>7</td><td>-9.4</td><td>20.072</td><td>23.086</td></tr> <tr><td>8</td><td>-9.4</td><td>19.634</td><td>20.348</td></tr> <tr><td>9</td><td>-9.4</td><td>4.921</td><td>9.414</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-10.0	0.000	0.000	2	-9.9	2.235	3.863	3	-9.8	27.078	28.146	4	-9.6	1.500	2.645	5	-9.4	20.786	23.827	6	-9.4	20.388	24.313	7	-9.4	20.072	23.086	8	-9.4	19.634	20.348	9	-9.4	4.921	9.414	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-8.8</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-8.6</td><td>14.681</td><td>17.252</td></tr> <tr><td>3</td><td>-8.6</td><td>5.016</td><td>9.777</td></tr> <tr><td>4</td><td>-8.5</td><td>15.971</td><td>20.283</td></tr> <tr><td>5</td><td>-8.5</td><td>17.171</td><td>21.023</td></tr> <tr><td>6</td><td>-8.4</td><td>15.962</td><td>21.314</td></tr> <tr><td>7</td><td>-8.4</td><td>6.223</td><td>9.005</td></tr> <tr><td>8</td><td>-8.4</td><td>24.266</td><td>27.084</td></tr> <tr><td>9</td><td>-8.4</td><td>1.168</td><td>1.821</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-8.8	0.000	0.000	2	-8.6	14.681	17.252	3	-8.6	5.016	9.777	4	-8.5	15.971	20.283	5	-8.5	17.171	21.023	6	-8.4	15.962	21.314	7	-8.4	6.223	9.005	8	-8.4	24.266	27.084	9	-8.4	1.168	1.821
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4	-8.5	15.971	20.283																																																																																
5	-8.5	17.171	21.023																																																																																
6	-8.4	15.962	21.314																																																																																
7	-8.4	6.223	9.005																																																																																
8	-8.4	24.266	27.084																																																																																
9	-8.4	1.168	1.821																																																																																
p-Menth-8-en-3-ol, acetate Present in AVSO	Compound CID: 94579	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-7.7</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-7.3</td><td>1.883</td><td>2.926</td></tr> <tr><td>3</td><td>-7.1</td><td>16.087</td><td>17.411</td></tr> <tr><td>4</td><td>-7.1</td><td>19.599</td><td>20.779</td></tr> <tr><td>5</td><td>-7.0</td><td>15.793</td><td>17.389</td></tr> <tr><td>6</td><td>-7.0</td><td>19.185</td><td>20.588</td></tr> <tr><td>7</td><td>-7.0</td><td>1.190</td><td>2.754</td></tr> <tr><td>8</td><td>-6.9</td><td>1.912</td><td>3.622</td></tr> <tr><td>9</td><td>-6.5</td><td>1.953</td><td>4.018</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-7.7	0.000	0.000	2	-7.3	1.883	2.926	3	-7.1	16.087	17.411	4	-7.1	19.599	20.779	5	-7.0	15.793	17.389	6	-7.0	19.185	20.588	7	-7.0	1.190	2.754	8	-6.9	1.912	3.622	9	-6.5	1.953	4.018	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-9.0</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-9.0</td><td>0.765</td><td>2.539</td></tr> <tr><td>3</td><td>-8.3</td><td>1.157</td><td>3.009</td></tr> <tr><td>4</td><td>-8.1</td><td>0.690</td><td>2.607</td></tr> <tr><td>5</td><td>-8.0</td><td>1.081</td><td>2.662</td></tr> <tr><td>6</td><td>-7.7</td><td>1.373</td><td>2.882</td></tr> <tr><td>7</td><td>-7.5</td><td>1.369</td><td>3.126</td></tr> <tr><td>8</td><td>-7.3</td><td>26.495</td><td>27.638</td></tr> <tr><td>9</td><td>-7.1</td><td>26.612</td><td>28.038</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-9.0	0.000	0.000	2	-9.0	0.765	2.539	3	-8.3	1.157	3.009	4	-8.1	0.690	2.607	5	-8.0	1.081	2.662	6	-7.7	1.373	2.882	7	-7.5	1.369	3.126	8	-7.3	26.495	27.638	9	-7.1	26.612	28.038
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Sclearal (sclareolide lactol) Present in AVSO	Compound CID: 537618	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-9.2</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-9.1</td><td>1.876</td><td>2.860</td></tr> <tr><td>3</td><td>-9.0</td><td>1.855</td><td>3.297</td></tr> <tr><td>4</td><td>-9.0</td><td>1.968</td><td>3.225</td></tr> <tr><td>5</td><td>-8.7</td><td>16.747</td><td>18.280</td></tr> <tr><td>6</td><td>-8.6</td><td>2.179</td><td>3.054</td></tr> <tr><td>7</td><td>-8.6</td><td>2.109</td><td>3.010</td></tr> <tr><td>8</td><td>-8.4</td><td>1.456</td><td>2.490</td></tr> <tr><td>9</td><td>-8.3</td><td>1.971</td><td>3.300</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-9.2	0.000	0.000	2	-9.1	1.876	2.860	3	-9.0	1.855	3.297	4	-9.0	1.968	3.225	5	-8.7	16.747	18.280	6	-8.6	2.179	3.054	7	-8.6	2.109	3.010	8	-8.4	1.456	2.490	9	-8.3	1.971	3.300	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-9.7</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-9.5</td><td>0.755</td><td>2.067</td></tr> <tr><td>3</td><td>-9.4</td><td>1.257</td><td>2.304</td></tr> <tr><td>4</td><td>-9.4</td><td>0.445</td><td>1.498</td></tr> <tr><td>5</td><td>-8.6</td><td>1.855</td><td>2.702</td></tr> <tr><td>6</td><td>-8.4</td><td>41.758</td><td>43.163</td></tr> <tr><td>7</td><td>-8.2</td><td>38.219</td><td>39.671</td></tr> <tr><td>8</td><td>-8.2</td><td>26.679</td><td>28.326</td></tr> <tr><td>9</td><td>-8.1</td><td>35.976</td><td>37.059</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-9.7	0.000	0.000	2	-9.5	0.755	2.067	3	-9.4	1.257	2.304	4	-9.4	0.445	1.498	5	-8.6	1.855	2.702	6	-8.4	41.758	43.163	7	-8.2	38.219	39.671	8	-8.2	26.679	28.326	9	-8.1	35.976	37.059
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12-Methyl-E,E-2,13-octadecadien-1-ol Present in AVSO	Compound CID: 90107969	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-6.4</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-6.3</td><td>1.751</td><td>2.345</td></tr> <tr><td>3</td><td>-6.3</td><td>1.604</td><td>1.826</td></tr> <tr><td>4</td><td>-6.2</td><td>15.600</td><td>18.215</td></tr> <tr><td>5</td><td>-5.9</td><td>28.748</td><td>30.594</td></tr> <tr><td>6</td><td>-5.9</td><td>8.383</td><td>8.840</td></tr> <tr><td>7</td><td>-5.7</td><td>28.457</td><td>30.471</td></tr> <tr><td>8</td><td>-5.6</td><td>15.740</td><td>17.193</td></tr> <tr><td>9</td><td>-5.5</td><td>4.031</td><td>8.362</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-6.4	0.000	0.000	2	-6.3	1.751	2.345	3	-6.3	1.604	1.826	4	-6.2	15.600	18.215	5	-5.9	28.748	30.594	6	-5.9	8.383	8.840	7	-5.7	28.457	30.471	8	-5.6	15.740	17.193	9	-5.5	4.031	8.362	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-7.0</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-7.0</td><td>3.939</td><td>6.577</td></tr> <tr><td>3</td><td>-6.3</td><td>24.797</td><td>26.149</td></tr> <tr><td>4</td><td>-6.0</td><td>36.786</td><td>38.971</td></tr> <tr><td>5</td><td>-5.6</td><td>3.829</td><td>8.991</td></tr> <tr><td>6</td><td>-5.5</td><td>15.114</td><td>18.852</td></tr> <tr><td>7</td><td>-5.5</td><td>14.853</td><td>16.227</td></tr> <tr><td>8</td><td>-5.4</td><td>37.260</td><td>40.258</td></tr> <tr><td>9</td><td>-5.3</td><td>20.346</td><td>21.671</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-7.0	0.000	0.000	2	-7.0	3.939	6.577	3	-6.3	24.797	26.149	4	-6.0	36.786	38.971	5	-5.6	3.829	8.991	6	-5.5	15.114	18.852	7	-5.5	14.853	16.227	8	-5.4	37.260	40.258	9	-5.3	20.346	21.671
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Phenol, 2,5-bis(1,1-dimethylethyl)- Present in AVSO	Compound CID: 79983	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-7.8</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-7.7</td><td>15.224</td><td>16.488</td></tr> <tr><td>3</td><td>-7.7</td><td>1.294</td><td>2.003</td></tr> <tr><td>4</td><td>-7.6</td><td>15.292</td><td>16.129</td></tr> <tr><td>5</td><td>-7.5</td><td>18.513</td><td>19.630</td></tr> <tr><td>6</td><td>-7.4</td><td>1.763</td><td>2.144</td></tr> <tr><td>7</td><td>-7.3</td><td>2.263</td><td>3.584</td></tr> <tr><td>8</td><td>-7.3</td><td>1.167</td><td>3.251</td></tr> <tr><td>9</td><td>-7.3</td><td>1.979</td><td>2.631</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-7.8	0.000	0.000	2	-7.7	15.224	16.488	3	-7.7	1.294	2.003	4	-7.6	15.292	16.129	5	-7.5	18.513	19.630	6	-7.4	1.763	2.144	7	-7.3	2.263	3.584	8	-7.3	1.167	3.251	9	-7.3	1.979	2.631	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-9.1</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-8.9</td><td>1.201</td><td>1.717</td></tr> <tr><td>3</td><td>-8.8</td><td>1.351</td><td>2.034</td></tr> <tr><td>4</td><td>-8.4</td><td>1.185</td><td>1.589</td></tr> <tr><td>5</td><td>-8.3</td><td>1.607</td><td>2.409</td></tr> <tr><td>6</td><td>-8.2</td><td>1.385</td><td>3.680</td></tr> <tr><td>7</td><td>-8.0</td><td>0.766</td><td>3.448</td></tr> <tr><td>8</td><td>-7.7</td><td>1.464</td><td>3.634</td></tr> <tr><td>9</td><td>-7.2</td><td>39.477</td><td>40.592</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-9.1	0.000	0.000	2	-8.9	1.201	1.717	3	-8.8	1.351	2.034	4	-8.4	1.185	1.589	5	-8.3	1.607	2.409	6	-8.2	1.385	3.680	7	-8.0	0.766	3.448	8	-7.7	1.464	3.634	9	-7.2	39.477	40.592
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2-Acetoxy-1,1,10-trimethyl-6,9-epidioxydecalin Present in AVSO	Compound CID: 538309	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-8.7</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-8.7</td><td>22.069</td><td>22.776</td></tr> <tr><td>3</td><td>-8.6</td><td>19.865</td><td>21.105</td></tr> <tr><td>4</td><td>-8.4</td><td>19.130</td><td>20.852</td></tr> <tr><td>5</td><td>-8.4</td><td>18.672</td><td>20.577</td></tr> <tr><td>6</td><td>-8.4</td><td>1.171</td><td>3.809</td></tr> <tr><td>7</td><td>-8.3</td><td>17.473</td><td>19.394</td></tr> <tr><td>8</td><td>-8.2</td><td>17.997</td><td>19.777</td></tr> <tr><td>9</td><td>-8.2</td><td>20.301</td><td>21.517</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-8.7	0.000	0.000	2	-8.7	22.069	22.776	3	-8.6	19.865	21.105	4	-8.4	19.130	20.852	5	-8.4	18.672	20.577	6	-8.4	1.171	3.809	7	-8.3	17.473	19.394	8	-8.2	17.997	19.777	9	-8.2	20.301	21.517	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-10.9</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-9.9</td><td>0.919</td><td>1.772</td></tr> <tr><td>3</td><td>-9.0</td><td>26.432</td><td>27.895</td></tr> <tr><td>4</td><td>-8.8</td><td>1.561</td><td>2.860</td></tr> <tr><td>5</td><td>-8.6</td><td>26.801</td><td>28.398</td></tr> <tr><td>6</td><td>-8.5</td><td>1.587</td><td>3.068</td></tr> <tr><td>7</td><td>-8.4</td><td>36.310</td><td>37.693</td></tr> <tr><td>8</td><td>-8.4</td><td>36.293</td><td>37.737</td></tr> <tr><td>9</td><td>-8.3</td><td>15.381</td><td>16.339</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-10.9	0.000	0.000	2	-9.9	0.919	1.772	3	-9.0	26.432	27.895	4	-8.8	1.561	2.860	5	-8.6	26.801	28.398	6	-8.5	1.587	3.068	7	-8.4	36.310	37.693	8	-8.4	36.293	37.737	9	-8.3	15.381	16.339
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5	-8.4	18.672	20.577																																																																																
6	-8.4	1.171	3.809																																																																																
7	-8.3	17.473	19.394																																																																																
8	-8.2	17.997	19.777																																																																																
9	-8.2	20.301	21.517																																																																																
mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.																																																																																
1	-10.9	0.000	0.000																																																																																
2	-9.9	0.919	1.772																																																																																
3	-9.0	26.432	27.895																																																																																
4	-8.8	1.561	2.860																																																																																
5	-8.6	26.801	28.398																																																																																
6	-8.5	1.587	3.068																																																																																
7	-8.4	36.310	37.693																																																																																
8	-8.4	36.293	37.737																																																																																
9	-8.3	15.381	16.339																																																																																

Compounds separated by GC-MS	Chemical (PubChem CID:)	AutoDock analysis results with 2rh1	AutoDock analysis results with 3D0G																																																																																
3H-3,10a-Methano-1,2-benzodioxocin-3-ol, octahydro-7,7-dimethyl-, (3.alpha.,6a.beta.,10a.beta.)- Present in AVSO	Compound CID: 606210	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-8.2</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-8.1</td><td>1.908</td><td>2.739</td></tr> <tr><td>3</td><td>-8.0</td><td>1.708</td><td>2.404</td></tr> <tr><td>4</td><td>-7.9</td><td>2.530</td><td>4.102</td></tr> <tr><td>5</td><td>-7.8</td><td>16.533</td><td>17.739</td></tr> <tr><td>6</td><td>-7.7</td><td>19.839</td><td>20.866</td></tr> <tr><td>7</td><td>-7.7</td><td>2.565</td><td>4.080</td></tr> <tr><td>8</td><td>-7.6</td><td>1.801</td><td>2.967</td></tr> <tr><td>9</td><td>-7.6</td><td>3.140</td><td>4.899</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-8.2	0.000	0.000	2	-8.1	1.908	2.739	3	-8.0	1.708	2.404	4	-7.9	2.530	4.102	5	-7.8	16.533	17.739	6	-7.7	19.839	20.866	7	-7.7	2.565	4.080	8	-7.6	1.801	2.967	9	-7.6	3.140	4.899	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-10.4</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-9.2</td><td>26.546</td><td>27.675</td></tr> <tr><td>3</td><td>-8.9</td><td>1.151</td><td>3.062</td></tr> <tr><td>4</td><td>-8.9</td><td>2.006</td><td>3.369</td></tr> <tr><td>5</td><td>-8.2</td><td>26.613</td><td>27.648</td></tr> <tr><td>6</td><td>-8.1</td><td>15.385</td><td>16.029</td></tr> <tr><td>7</td><td>-8.0</td><td>15.591</td><td>16.196</td></tr> <tr><td>8</td><td>-7.7</td><td>36.293</td><td>37.528</td></tr> <tr><td>9</td><td>-7.6</td><td>14.872</td><td>15.634</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-10.4	0.000	0.000	2	-9.2	26.546	27.675	3	-8.9	1.151	3.062	4	-8.9	2.006	3.369	5	-8.2	26.613	27.648	6	-8.1	15.385	16.029	7	-8.0	15.591	16.196	8	-7.7	36.293	37.528	9	-7.6	14.872	15.634
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Tricyclo[4.3.0.0(7,9)]nonane, 2,2,5,5,8,8-hexamethyl-, (1.alpha.,6.beta.,7.alpha.,9.alpha.)- Present in AVSO	Compound CID: 549738	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-8.8</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-8.8</td><td>0.013</td><td>2.288</td></tr> <tr><td>3</td><td>-8.6</td><td>0.603</td><td>2.758</td></tr> <tr><td>4</td><td>-8.6</td><td>0.603</td><td>3.419</td></tr> <tr><td>5</td><td>-8.5</td><td>18.565</td><td>20.238</td></tr> <tr><td>6</td><td>-8.5</td><td>18.564</td><td>20.256</td></tr> <tr><td>7</td><td>-8.4</td><td>9.193</td><td>9.765</td></tr> <tr><td>8</td><td>-8.3</td><td>9.140</td><td>9.919</td></tr> <tr><td>9</td><td>-8.3</td><td>9.792</td><td>10.512</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-8.8	0.000	0.000	2	-8.8	0.013	2.288	3	-8.6	0.603	2.758	4	-8.6	0.603	3.419	5	-8.5	18.565	20.238	6	-8.5	18.564	20.256	7	-8.4	9.193	9.765	8	-8.3	9.140	9.919	9	-8.3	9.792	10.512	<table> <tr> <th>mode</th><th>affinity (kcal/mol)</th><th>dist from best mode rmsd l.b.</th><th>rmsd u.b.</th></tr> <tr><td>1</td><td>-10.8</td><td>0.000</td><td>0.000</td></tr> <tr><td>2</td><td>-10.8</td><td>0.067</td><td>2.289</td></tr> <tr><td>3</td><td>-10.6</td><td>0.645</td><td>2.674</td></tr> <tr><td>4</td><td>-10.6</td><td>0.646</td><td>3.085</td></tr> <tr><td>5</td><td>-10.0</td><td>0.608</td><td>2.931</td></tr> <tr><td>6</td><td>-8.9</td><td>1.263</td><td>2.904</td></tr> <tr><td>7</td><td>-8.4</td><td>35.486</td><td>37.153</td></tr> <tr><td>8</td><td>-7.9</td><td>35.545</td><td>37.763</td></tr> <tr><td>9</td><td>-7.6</td><td>15.022</td><td>16.026</td></tr> </table>	mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.	1	-10.8	0.000	0.000	2	-10.8	0.067	2.289	3	-10.6	0.645	2.674	4	-10.6	0.646	3.085	5	-10.0	0.608	2.931	6	-8.9	1.263	2.904	7	-8.4	35.486	37.153	8	-7.9	35.545	37.763	9	-7.6	15.022	16.026
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Table 9: Results of the GC-MS analysis of the studied seed extracts (GSO, PSO, ASO, AWSO, PGSO and AVSO) with the AutoDock analysis as potential ligand binding to the $\beta 2$ adrenoceptor (2rh1) and ACE2 receptor (3D0G).

Compounds	Chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole) with 2rh1 with the best enlarged angle for ligand with the protein	Global binding energy of the highest binding affinity (kcal/mole) with 3D0G with the best enlarged angle for ligand with the protein
9-Octadecenamide, (Z)- Or Oleamide Present in all(GSO, PSO, ASO, AWSO, PGSO, AVSO)	Compound CID: 5283387 MF: C18H35NO	-7.9	-8.7

Compounds	Chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole) with 2rh1 with the best enlarged angle for ligand with the protein	Global binding energy of the highest binding affinity (kcal/mole) with 3D0G with the best enlarged angle for ligand with the protein
Stigmastan-3,5-diene Present in (GSO, PSO, AWSO, PGSO, AVSO)	Compound CID: 525918 MF: C ₂₉ H ₄₈	-11.4	-11.6
Hexadecanamide Present in all(GSO, PSO, ASO, AWSO, PGSO, AVSO)	Compound CID: 69421 MF: C₁₆H₃₃NO	-6.6	-7.7
Pentanoic acid, 5-hydroxy-, 2,4-di-t-butylphenyl esters Present in GSO, PSO, PGSO	Compound CID: 605777 MF: C ₁₉ H ₃₀ O ₃	-10.2	-10.1

Compounds	Chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole) with 2rh1 with the best enlarged angle for ligand with the protein	Global binding energy of the highest binding affinity (kcal/mole) with 3D0G with the best enlarged angle for ligand with the protein
Methyl stearate GSO, PSO ONLY	Compound CID: 8201 MF: C ₁₉ H ₃₈ O ₂	-6.0	-5.7
1,3-Benzenediol, o-(4-methylbenzoyl)-o'-(2-methoxybenzoyl)- Present in GSO, PSO ,ONLY	Compound CID: 91715040 MF: C ₂₂ H ₁₈ O ₅	-10.3	-9.5
2-Bromotetradecane GSO, AVSO ONLY	Compound CID: 12798926 MF: C₁₄H₂₉Br	-5.4	-6.1

Compounds	Chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole) with 2rh1 with the best enlarged angle for ligand with the protein	Global binding energy of the highest binding affinity (kcal/mole) with 3D0G with the best enlarged angle for ligand with the protein
Isooctyl 3-mercaptopropionate GSO ONLY	Compound CID: 104386 MF: C₁₁H₂₂O₂S	-6.4	-7.2
Squalene Present in(PSO, ASO, AWSO, PGSO, AVSO	Compound CID: 638072 MF: C₃₀H₅₀	-10.6	-9.7
Propanoic acid, 3-mercapto-, dodecyl ester Present in GSO, AVSO	Compound CID: 80796 MF: C₁₅H₃₀O₂S	-6.7	-6.5

Compounds	Chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole) with 2rh1 with the best enlarged angle for ligand with the protein	Global binding energy of the highest binding affinity (kcal/mole) with 3D0G with the best enlarged angle for ligand with the protein
1,2-15,16-Diepoxyhexadecane	Compound CID: 543423 MF: C₁₆H₃₀O₂	-5.8	-6.3
cis-Vaccenic acid ASO ONLY	Compound CID: 5282761 MF: C ₁₈ H ₃₄ O ₂	-8.2	-9.3
cis-11-Eicosenamide Present in (ASO, AWSO, PGSO, AVSO)	Compound CID: 5365374 MF: C₂₀H₃₉NO	-7.5	-7.5

Compounds	Chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole) with 2rh1 with the best enlarged angle for ligand with the protein	Global binding energy of the highest binding affinity (kcal/mole) with 3D0G with the best enlarged angle for ligand with the protein
2-Furancarboxaldehyde, 5-methyl- Present in (ASO)only	Compound CID: 12097 MF: C₆H₆O₂	-5.2	-5.5
dl-.alpha.-Tocopherol Present in (ASO, AVSO)	Compound CID: 2116 MF: C₂₉H₅₀O₂	-10.2	-9.2
4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- Present in (ASO, AWSO)	Compound CID: 119838 MF: C ₆ H ₈ O ₄	-5.5	-5.5

Compounds	Chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole) with 2rh1 with the best enlarged angle for ligand with the protein	Global binding energy of the highest binding affinity (kcal/mole) with 3D0G with the best enlarged angle for ligand with the protein
5-Hydroxymethylfurfural Present in (AWSO)	Compound CID: 237332 MF: C₆H₆O₃	-5.2	-5.8
Oleic Acid Present in AWSO, AVSO	Compound CID: 445639 MF: C ₁₈ H ₃₄ O ₂	-6.9	-7.5
.alpha.-D-Glucopyranoside, O-.alpha.-D-glucopyranosyl- (1.fwdarw.3)-.beta.-D- fructofuranosyl Present in AWSO	Compound CID: 220003 MF: C₁₈H₃₂O₁₆	-9.0	-9.2

Compounds	Chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole) with 2rh1 with the best enlarged angle for ligand with the protein	Global binding energy of the highest binding affinity (kcal/mole) with 3D0G with the best enlarged angle for ligand with the protein
Palmitic Acid Present in AWSO	Compound CID: 985 MF: C16H32O2	-6.2	-6.8
Levoglucosenone Present in AWSO	Compound CID: 699486 MF: C6H6O3	-4.8	-5.5
Cyclopropanecarboxylic acid, 3-formyl-2,2-dimethyl-, ethyl ester Present in AWSO	Compound CID: 566079 MF: C9H14O3	-5.5	-5.9

Compounds	Chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole) with 2rh1 with the best enlarged angle for ligand with the protein	Global binding energy of the highest binding affinity (kcal/mole) with 3D0G with the best enlarged angle for ligand with the protein
1H-Inden-1-ol, 2,3-dihydro- Present in AWSO	Compound CID: 22819 MF: C ₉ H ₁₀ O	-6.4	-8.1
Phenol, 2,6-bis(1,1-dimethylethyl)- Present in AWSO	Compound CID: 31405 MF: C₁₄H₂₂O	-7.5	-9.2
Chloro(2-methyloxiran-2-yl)acetic acid, t-butyl ester Present in AWSO	Compound CID: 545402 MF: C₉H₁₅ClO₃	-6.1	-6.6

Compounds	Chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole) with 2rh1 with the best enlarged angle for ligand with the protein	Global binding energy of the highest binding affinity (kcal/mole) with 3D0G with the best enlarged angle for ligand with the protein
Cyclodecacyclododecene, 1,2,3,4,5,6,7,8,9,10,11,12,13, 14,15,16,17,18-octadecahydro-	Compound CID: 5377998 MF: C ₂₀ H ₃₆	-10.2	-10.9
2H-Pyran, 2-(7-heptadecynyloxy)tetrahydro-	Compound CID: 543312 MF: C₂₂H₄₀O₂	-6.6	-6.2
Androstan-17-one, 3-ethyl-3-hydroxy-, (5.alpha.)-	Compound CID: 14681481 MF: C₂₁H₃₄O₂	-10.7	-11.5

Compounds	Chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole) with 2rh1 with the best enlarged angle for ligand with the protein	Global binding energy of the highest binding affinity (kcal/mole) with 3D0G with the best enlarged angle for ligand with the protein
Z,E-2,13-Octadecadien-1-ol	Compound CID: 5364462 MF: C ₁₈ H ₃₄ O	-6.7	-6.9
Chrysene, octadecahydro	Compound CID: 98460 MF: C₁₈H₃₀	-9.6	-11.5
Bicyclo[10.6.0]octadec-1(12),15-diene	Compound CID: 5362802 MF: C₁₈H₃₀	-9.2	-10.6

Compounds	Chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole) with 2rh1 with the best enlarged angle for ligand with the protein	Global binding energy of the highest binding affinity (kcal/mole) with 3D0G with the best enlarged angle for ligand with the protein
3-Chloropropionic acid, heptadecyl ester	Compound CID: 545757 MF: C ₂₀ H ₃₉ ClO ₂	-7.4	-6.8
1-Heptatriacotanol	Compound CID: 537071	-5.3	-4.6
13-Docosenamide, (Z)-	Compound CID: 5365371 MF: C ₂₂ H ₄₃ NO	-8.8	-8.6

Compounds	Chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole) with 2rh1 with the best enlarged angle for ligand with the protein	Global binding energy of the highest binding affinity (kcal/mole) with 3D0G with the best enlarged angle for ligand with the protein
Caryophyllene oxide	Compound CID: 1742210 MF: C₁₅H₂₄O	-8.6	-10.4
Heptacosane	Compound CID: 11636 MF: C₂₇H₅₆	-5.9	-5.0
.gamma.-Tocophero	Compound CID: 91738518 MF: C ₃₀ H ₄₇ F ₃ O ₃	-10.0	-8.8

Compounds	Chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole) with 2rh1 with the best enlarged angle for ligand with the protein	Global binding energy of the highest binding affinity (kcal/mole) with 3D0G with the best enlarged angle for ligand with the protein
p-Menth-8-en-3-ol, acetate	Compound CID: 94579 MF: C ₁₂ H ₂₀ O ₂	-7.7	-9.0
Scarlal (sclareolide lactol)	Compound CID: 537618 MF: C₁₆H₂₈O₂	-9.2	-9.7
12-Methyl-E,E-2,13-octadecadien-1-ol	Compound CID: 90107969 MF: C₁₉H₃₆O	-6.4	-7.0

Compounds	Chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole) with 2rh1 with the best enlarged angle for ligand with the protein	Global binding energy of the highest binding affinity (kcal/mole) with 3D0G with the best enlarged angle for ligand with the protein
Phenol, 2,5-bis(1,1-dimethylethyl)-	Compound CID: 79983	-7.8	-9.1
2-Acetoxy-1,1,10-trimethyl-6,9-epidioxydecalin	Compound CID: 538309 MF: C₁₅H₂₄O₄	-8.7	-10.9
3H-3,10a-Methano-1,2-benzodioxocin-3-ol, octahydro-7,7-dimethyl-, (3.alpha.,6a.beta.,10a.beta.)-	Compound CID: 606210 MF: C₁₃H₂₂O₃	-8.2	-10.4

Compounds	Chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole) with 2rh1 with the best enlarged angle for ligand with the protein	Global binding energy of the highest binding affinity (kcal/mole) with 3D0G with the best enlarged angle for ligand with the protein
Tricyclo[4.3.0.0(7,9)]nonane, 2,2,5,5,8,8-hexamethyl-, (1.alpha.,6.beta.,7.alpha.,9.alpha.)-	Compound CID: 549738 MF: C₁₅H₂₆	-8.8	-10.8
Synergetic		Mean =7.66	Mean =-8.35

Table 10: Prediction of the best interaction of the ligands of GSO, PSO, ASO, AWSO, PGSO and AVSO with $\beta 2$ adrenoreceptor (2rh1) and ACE2 receptor (3D0G) in the AutoDock analysis.

Discussion

The coronavirus pandemic has had many consequences, including health, psychological and economic consequences. The World Health Organization approved a group of drugs to treat the virus. Besides the drugs, there are ongoing races in production of vaccines. Furthermore, scientists are increasingly focusing their efforts to discover vaccines without side effects. However, the discovery of novel coronavirus mutations requires more attention and

considerations and varied drugs and vaccine proposals; for example, phytochemistry potential trials.

Phytochemicals in fruits, vegetables and plant parts hold secondary metabolites and their essential metabolites have several inherent biological activities that involve antimicrobial, anti-inflammatory and inhibitory enzyme properties with health benefits [30,31]. In our previous studies, avocado and pomegranate juice, peel and seed oil ameliorated toxicity and decreased inflammation, oxidative stress and apoptosis induced by CCl₄ and DEN [21,32-35].

Grape (*Vitis vinifera*) was introduced to the literature as a treatment after an Arab doctor suggested it as a royal oil for skin treatment for Ferdinand IV in the 14th century. It also has antioxidant and anti-inflammatory properties, according to the previous investigation. The seed composition of fruits depends on maturation, the environmental cultivation state and extraction protocol [36-38]. The results of the current study's seed extract analysis (Table 1-7) showed that Grape Seed Oil (GSO) included 9-octadecenamide, (z)-, stigmastan-3, 5-diene, 9, 12-octadecadienoic acid (z, z)-, methyl ester, oleamide, hexadecanamide and phosphoric acid trimethyl ester. Furthermore, GSO was found to contain dodecyl acrylate, pentanoic acid, 5-hydroxy-, 2,4-di-*t*-butylphenyl esters, methyl stearate and 1-pentadecyne. It also included 1-pentadecyne, 11, 13-dimethyl-12-tetradecen-1-ol acetate, 4-methyl-2,4-bis(4'-trimethylsilyloxyphenyl)pentene-1, 1,3-benzenediol, *o*-(4-methylbenzoyl)-*o*'-(2-methoxybenzoyl)-, 2-bromotetradecane, cyclotrisiloxane, hexamethyl- and isooctyl 3-mercaptopropionate (Table 1).

GSO compositions such as 9-octadecenamide, (z)-, 9,12-octadecadienoic acid (z, z)-, oleamide and hexadecanamide have a sedative effect where a group of an amide of the fatty acid oleic acid is located as naturally endogenous on the animal's body. It has an accumulation function in the cerebrospinal fluid during sleep deprivation and influences animal's sleep, making those oleamide derivatives potential treatments for mood, depression and sleep disorders through interaction with multiple neurotransmitters. Further, it binds the Cannabinoid receptor type 1 (CB1) receptor as a full agonist. Also, these derivatives have anti-corrosive properties [39-42]. Stigmastane, 24R-ethylcholestane, is a tetracyclic triterpene and cholestane as well as ergostane. This sterane is applied as a biomarker for initial eukaryotes. Stigmastanol, Stigmastan-3, 5-diene and their derivatives are types of plant phytosterol that inhibit cholesterol absorption from the diet [43]. Acrylates are the salts, esters and conjugate bases of acrylic acid, including dodecyl acrylate, for example. They have various bifunctional functionalities such as in the polymers industry and as antimicrobial and non-chemical based antioxidant agents [44-46]. GSO also contains phosphoric acids that are not genotoxic nor carcinogenic and is therefore used as a food additive in water treatment products. Further, it is used as phosphate salts for fertilizers, dental cement, albumin derivatives and the sugar and textile industries [47].

GSO contains a group of ester, acetate and valeric or pentanoic acids; all have pleasant odors and are used in the perfume and cosmetic additives industry. Valeric acid is a minor product of

the gut microbiome and can also be produced by its esters' metabolism found in food [48,49]. The repair of these acid levels in the gut has been recommended as the mechanism in the govern of the clostridioides difficile infection after fecal microbiota transplant [49].

Methyl stearate is a fatty acid methyl ester and octadecanoate ester. Stearic acid has a role as a metabolite and is connected with reduced LDL cholesterol compared to other saturated fatty acids. It is used in lubricants, detergents, softening agents, release agents and food additives, as well as in batteries and electronic devices [50,51].

GSO contains different bioactive secondary metabolites such as sulfurous acid, 2-ethylhexyl isohexyl ester, heptacosane, dodecyl pentyl ester, eicosane 2- methyl, benzyl detervitive and 2-bromotetradecane, dodecyl acrylate as well as 1,3-benzenediol, o-(4-methylbenzoyl)-o'-(2-methoxybenzoyl)-. These combinations of secondary metabolites are related to antibacterial, antifungal and anti-diabetic attributes [52-55]. Other metabolites such as 4-methyl-2, 4-bis (4-hydroxyphenyl) pent-1-ene (MBP) have potent estrogenic action *in-vitro* and *in-vivo*; moreover, computer modelling has revealed that this greater strength is due to more effective binding to estrogen receptors. Previous studies reported that cyclotrisiloxane and hexamethyl-derivatives have antioxidant and antibacterial activity. GSO contains isooctyl 3-mercaptopropionate that depravities reported antioxidant and anti-inflammatory [56-59].

A plum is a fruit of a unique species, *Prunus subg. Prunus*. Plum stones include a seed with a high content of proteins and lipids that are frequently underused and undervalued. Victoria Plum Seed Oil extract (PSO) includes phytosterols such as stigmastan-3, 5-diene and hexadecanamide derivatives also found in current grape seed extract (Table 2). PSO contains esters, methyl stearate, dodecyl acrylate and benzyl detectives, which have beneficial antibacterial, anti-inflammatory, anticancer and antioxidant effects, as was discussed before concerning grape seed oil extract with the relative value of RT: Retention Times (minutes). PSO comprises squalene, a natural organic polyunsaturated hydrocarbon of the triterpene type know as shark liver oil. All plants, animals, birds and human livers provide squalene as a biochemical intermediate. It preserves polyunsaturated fatty acids against temperature-dependent autoxidation. Squalene also functions essentially as a peroxy radical scavenger, is useful for skin hydration, works as an antioxidant, has antitumor properties and is used in cosmetics [60,61].

Apple seeds are rich in proteins, carbohydrates and minerals, making them useful as feed or fertilizer [62]. Moreover, they contain fatty linoleic acid, sterols, tocopherols, a primary fatty amid cis-11-eicosenamide and hydrocarbons, especially squalene 63, which is confirmed by the present study's apple seed oil GC-MS analysis. Previous investigations reported that apple seed oil can improve the treatment of various diseases, especially Cardiovascular Disease (CVD) and diabetic disorder. This improvement is effected by managing the blood lipid profile, blood pressure, adipocyte hormones, inflammatory response, endothelial capacity and through numerous other beneficial effects as anticancer, antioxidant and antibacterial properties

[64,65]. Moreover, dl- α -tocopherol (vitamin E) was reported as an antidepressant and significant antioxidant [63-65]. Apple Seed Oil (ASO) contains hexadecanamide, benzoic acid fatty acid esters and -octadecenoic acid and their derivatives, which have beneficial antibacterial, anti-inflammatory, anticancer and antioxidant effects, as discussed before regarding grape seed oil and plum seed oil. Apple seeds oil, also rich in fatty acids such as vaccenic acid, is an omega-7 fatty acid with antibacterial, antioxidant and anti-coronary heart disease properties [66,67]. ASO includes 2-pyrrolidinovalerophenone, which is used as a bath salt and has a neurological effect and 2-furancarboxaldehyde, 5-methyl-F, which is a derivative inhibiting sickle cell formation in the blood.

Additionally, it contains radical scavenging activity compounds such as 13-Tetradecenal. This is because plum, grape and apple seeds have a phenolic composition with antioxidant capacity, comprising 4H-pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- and 9,12-octadecadienoic acid (Z, Z)- and phenylmethyl ester [68-71].

Date palm (*Phoenixdactylifera*) is a member of the palm family (Arecaceae) and has been used as food for over 6000 years. It is found in Saudi Arabia, Middle Eastern countries and Egypt. Its components such as carbohydrates, phytochemicals, sterols, carotenes and flavonoids have been screened for numerous therapeutic activities and are found to decrease the side effects of manufactured medicines that hurt the human biological system. Besides, date seeds are used as animal feed or caffeine-free coffee replacements in some areas. The Ajwa date seed oil includes sterol, phytochemistry, oleic, palmitic and fatty acids and their derivatives; these have antibacterial, antioxidant, anticancer and antilipidemic effects [72,73]. The present work reported that Ajwa date seed oil (AWSO) contains hexadecanamide, 5-hydroxymethylfurfura, 9-octadecenamide, (Z)-, oleic acid, cis-11-eicosenamide, dodecanoic acid and palmitic acid. Squalene and stigmastan-3,5-diene are found in it. AWSO contains fatty acid ester, other phenol and furfural derivatives, as presented in Table 4. These compounds have antioxidant and anti-inflammatory, neurological, sedation and cosmetic effects. Moreover, it contains 7-methyl-Z-tetradecen-1-ol acetate, which has the effect of heat and heat cough [74].

The present work reported that pomegranate (*Punica granatum L.*), which belongs to the Punicaceae family (PGSO), contains hexadecanamide, 5-hydroxymethylfurfural, 9-octadecenamide, (Z)-, oleamide, cis-11-eicosenamide, dodecyl acrylate and fatty acid ester, as well as phenol, squalene, stigmastan-3,5-diene (Table 5). These compounds have antioxidant and anti-inflammatory effects [19]. Avocados (*Persea Americana*) are related to the Lauraceae family. Avocados contain carotenoids, minerals, phenolics, vitamins and fatty acids. Further, avocados have lipid-lowering, antihypertensive, antidiabetic, anti-obesity, antithrombotic, antiapoptosis and anti-atherosclerotic cardio-protective effects. The avocado seeds are considered one of the fruit's non-edible parts, which are generally discarded as trash and can cause environmental problems. Examining such foods' underutilized dietary and therapeutic potential will also diminish the environmental waste load [33,75].

The composition of avocado seed includes protein, fat, ash, moisture, fiber and carbohydrate, minerals such as Ca, Zn, K, Na, P, Fe, Cu, Pb and Co) phytochemicals (flavonoid, tanine, saponine, total phenolics, antioxidant capacity, oxalates, phytates and alkaloids) and vitamins (A, B1, B2, B3, C and E). The avocado seeds have antioxidant and antimicrobial, antihypertensive, fungicidal, larvicidal, hypolipidemic, amoebicidal and giardicidal activities [76].

The present study indicated that AVSO contains many fatty acids and their derivatives (Table 6), such as linoleyl alcohol and carboxamide derived from palmitic acid and volatile compounds, for example, cyclodecacyclododecene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18-octadecahydro-, hexadecanamide, 9-octadecenamide, (Z)-, 2H-pyran and 2-(7-heptadecynyloxy)tetrahydro. AVSO includes steroids such as androstan-17-one, 3-ethyl-3-hydroxy-, (5.alpha.) and the polycyclic aromatic hydrocarbon chrysene, octadecahydro. Also, its composition of 11-eicosenoic acid, monounsaturated omega-9 fatty, dl.alpha.-tocopherol and gamma.-tocophero shows antioxidant activity. AVSO includes bicyclic organic compounds such as bicyclo[10.6.0]octadeca-1(12),15-diene as well as antitumor cis-10-nonadecenoic acid, monounsaturated fatty cis-10-nonadecenoic acid [77-79].

AVSO contains many essential and volatile oils, ester derivatives, farnesol isomer, heptacosane and 3-chloropropionic acid, heptadecyl este. Caryophyllene oxide has chemopreventative, anti-tumor and antifungal properties and is used in approved food flavoring and other benzyl, organic and aromatic derivatives, as indicated in Table 6 [80,81]. It yields antioxidant compounds such as oleic acid, stigmastan-3,5-diene and antifungal cosmetics agents such as sclaral (sclareolide lactol) [82].

Molecular docking is a theoretical simulation system based on bioinformatics, which depends on the cooperation between molecules (such as ligands and receptors) and predicts their binding modes and affinity by computer investigation. Molecular docking works as an acceptable tool in medicinal chemistry for fields such as structure-based analytical drugs. Various original studies corresponding to biomolecular cooperation in food pattern and phytochemistry have continuously evolved. The remarkable benefits of molecular docking, such as predicting procedures with fewer experiments and limiting the decline of material in trials, have led to the consideration of its possible administration in various areas. In docking complex binding energy, the lowest energy positions designate the highest binding affinity, as high energy creates variable conformations that assist in pharmacological experiments. Our previous work on rat and human investigations showed that the treatment effect of vitamin B and agarwood extracts confirmed by molecular docking might be due to their role as inverse agonists, reversing the induction of stress and depression by epinephrine with many medicinal properties, such as sedative, anti-inflammatory and anti-apoptotic effects [10]. The present work described the investigated compounds in the seed extracts have a potential binding mode

with the $\beta 2$ adrenoreceptor (2rh1) and ACE2 receptor (3D0G) by docking analysis (Table 9,10). Further, the inhibitory effect of synergetic extract compounds was also reported. The present finding established the seed compounds' ameliorating effect against both studied receptors and might represent the studied extract as an inverse agonist ligand for depression and infection in the COVID-19 pandemic.

We have future application possibilities in using the currently investigated seed oil extracts in manufacture as endogenous nanoparticles as drugs carrier or vaccines to target cell receptors and prolong their circulation time. Moreover, as the seed oil extract is present in fruit and is edible, it will help decrease the side effects that are likely to occur due to nanoparticles, vaccines and drugs in the surrounding and body tissue.

Many bioactive phytochemicals and herbal medicines have low solubility in aqueous media, poor bioavailability, poor stability and toxicity-dose dependence, so scientists have used nanotechnology to overcome these disadvantages and deliver bioactive phytochemicals to the target with higher efficiency, using encapsulation. For this goal, nanoparticles can be provided in various forms, sizes and combinations and adjusted physicochemically to accomplish particular characteristics, depending on the features of both the bioactive molecule and the target cell, such as an inorganic gold atom (molecular weight = 196.96657 g/mol) or organic liposome (molecular weight = 938.1 g/mol). Unfortunately, there are challenges such as the potential toxicity of nanoparticles, such as immunotoxicity, the toxicity of surfactants and co-surfactants or emulsifier nanocarriers, long-term toxicity due to chronic exposure and the accumulation as well as overaccumulation of nanoparticles at all barriers before acting on the targeted cells. The analyzed seed oil contents' binding energy with the currently studied receptors enables them to be future nanoparticles in vaccines and drugs. Further, the molecular weight allows them to be nanocarriers [83-86].

Conclusion

In this investigation, the binding interactions of 44 phytoconstituents were carried out against the $\beta 2$ adrenoreceptor (2rh1) and the ACE2 receptor, 3D0G. All the currently studied seed oil extract constituent were identified by gas chromatography-mass spectrometry and studied. The present investigation strongly suggests the application of these seed oil extracts to ameliorate depression and decrease and prevent infection in the COVID pandemic. Further studies need to be carried out to examine these compounds' pharmacological properties and inhibitory potentials require experimental models.

Author Contributions

A.F.H. contributed to creating and owning, conceptualizing, work idea designing and performing the experiments, chromatography and AutoDock analysis, interpreting and analyzing data, writing, revising and editing the manuscript and explaining the results. T.M.F. contributed to the AutoDock analysis and formatting manuscript. I.M.A, I.A.K, M.E.O, M.A.A and F.M.A. contributed to the doing practical of the chromatography portion of the study.

Ethical Statement

This research did not include any human subjects or animal experiments.

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